=> d his

(FILE 'HOME' ENTERED AT 09:59:03 ON 27 DEC 2007)

FILE 'REGISTRY' ENTERED AT 10:00:33 ON 27 DEC 2007

L1 STRUCTURE UPLOADED

L2 12 S L1

L3 282 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:01:14 ON 27 DEC 2007

L4 146 S L3

FILE 'REGISTRY' ENTERED AT 10:03:52 ON 27 DEC 2007

L5 STRUCTURE UPLOADED

L6 19 S L5

L7 STRUCTURE UPLOADED

L8 19 S L7

L9 66913 S CAN

FILE 'REGISTRY' ENTERED AT 11:05:04 ON 27 DEC 2007

L10 19 S L7

L11 261 S L7 FUL

L12 6 SEARCH L7 CSS SUB=L11 FUL

FILE 'CAPLUS' ENTERED AT 11:07:27 ON 27 DEC 2007

L13 3 S L12

=> d bib abs hitstr 1-3

L13 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1986:148472 CAPLUS

DN 104:148472

TI Synthesis of amine derivatives

IN Masuko, Fujio; Katsura, Tadashi

PA Sumitomo Chemical Co., Ltd., Japan

SO U.S., 13 pp. Cont.-in-part of U.S. Ser. No. 65,429, abandoned. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

PAN.	FAN.CNI 2						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	US 4536599	A	19850820	US 1979-90479	19791101		
	JP 55028959	Α	19800229	JP 1978-102614	19780822		
	JP 61055488	В	19861128				
	JP 55033442	Α	19800308	JP 1978-106541	19780830		
	JP 62000905	В	19870110				
PRAI	JP 1978-102614	A	19780822				
	JP 1978-106541	Α	19780830				
	US 1979-65429	A2	19790810				
os	MARPAT 104:148472						
GI			•				

$$R^{1}$$
 (CHR³) n CHR R^{4}

chain nodes:

2 3 15 16 17 19 20 21 22 23 24 25 29 31 ring nodes:

1 4 5 6 7 8 9 10 11 12 13 14

chain bonds:

1-2 2-3 2-19 3-4 3-15 15-16 15-17 20-21 20-22 23-24 24-25 ring bonds :

1-5 1-9 4-10 4-14 5-6 6-7 7-8 8-9 10-11 11-12 12-13 13-14

₃3:3 E exact RC ring/chain

Match level:

1:Atom 2:CLASS3:CLASS4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:/ 13:Atom 14:Atom 15:CLASS16:CLASS17:CLASS19:CLASS20:CLASS2 24:CLASS25:CLASS29:CLASS30:Atom 31:CLASS32:Atom

Diphenylalkylamines I (R = NH2; R1-R5 = H, halo, OH, trihalomethyl, Ph, PhO, PhS, alkyl, alkenyl, alkoxy, alkylthio, dialkylamino, alkylsulfonyl; n = 2, 3), useful as pharmaceutical intermediates and optical resolution agents, were prepared by condensing R4R5C6H3CH2CN with R1R2C6H3(CHR3)nX (X = halo) in the presence of a base, hydrolysis of the resultant I (R = cyano) by H2O2 and a base in the presence of an organic quaternary ammonium salt, and Hofmann rearrangement of the resultant I (R = CONH2) in the presence of a base. Thus, 4-C1C6H4CH2CN, PhCH2Cl, Bu4NBr, and 25% aqueous NaOH reacted in PhMe to give 95% PhCH2CHRC6H4Cl-4 (II; R = cyano), which was hydrolyzed by aqueous NaOH-H2O2 in MeOH in the presence of Bu4NBr to give 98% II (R = CONH2). Rearrangement of the amide by Br-NaOH in MeOH gave 97% II (R = NH2) (III), which was resolved by L-(+)-tartaric acid to give 50% resolution yield of 1-III.

IT 74533-40-7P 74533-41-8P 74533-42-9P

74533-47-4P 74533-54-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with hypohalite)

RN 74533-40-7 CAPLUS

CN Benzenepropanamide, 4-methyl $-\alpha$ -(4-methylphenyl)- (CA INDEX NAME)

RN 74533-41-8 CAPLUS

CN Benzenepropanamide, α -(4-chlorophenyl)-4-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ &$$

RN 74533-42-9 CAPLUS

CN Benzenepropanamide, α-(3-bromophenyl)-4-methyl- (CA INDEX NAME)

RN 74533-47-4 CAPLUS

CN Benzenepropanamide, α -(3-hydroxyphenyl)-4-propyl- (CA INDEX NAME)

RN 74533-54-3 CAPLUS

CN Benzenepropanamide, 2-ethyl- α -(3-methylphenyl)- (CA INDEX NAME)

L13 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1983:575329 CAPLUS

DN 99:175329

OREF 99:26889a,26892a

TI Oxidative decyanation of benzyl and benzhydryl cyanides. A simplified procedure

AU Kulp, Stuart S.; McGee, Michael J.

CS Dep. Chem., Moravian Coll., Bethlehem, PA, 18018, USA

SO Journal of Organic Chemistry (1983), 48(22), 4097-8

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 99:175329

AB The reaction of 24 examples of mono and disubstituted nitriles with atmospheric oxygen in Me2SO and either K2CO3 or lithium isopropylcyclohexylamide base at ambient temperature is reported. In 13 cases the oxidative decyanation product (ketone) was obtained in >90% yield. Thus, 1.00 g PhCH2CN was treated with 1.00 g K2CO3 in 30 mL Me2SO at room temperature to give 0.809 Ph2CO

(95% yield). Reaction half-lifes were determined for several nitriles.

IT 87184-36-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, by oxidative decyanation of nitrile)

RN 87184-36-9 CAPLUS

CN Benzenepropanamide, α -(4-chlorophenyl)-4-methoxy- (CA INDEX NAME)

L13 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1980:495018 CAPLUS

DN 93:95018

OREF 93:15221a,15224a

II Synthesis of amides and amines

IN Masuko, Fujio; Katsura, Tadashi

PA Sumitomo Chemical Co., Ltd., Japan

SO Eur. Pat. Appl., 49 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 2

T. Tara	CIVI Z			
	PATENT NO.	KIND DATE	APPLICATION NO.	DATE
ΡI	EP 8532	A1 19800305	EP 1979-301696	19790820
	EP 8532	B1 19830720		
	R: BE, CH, DI	E, FR, GB, IT, NL,	SE	
	JP 55028959	A 19800229	JP 1978-102614	19780822
	JP 61055488	B 19861128		
	JP 55033442	A 19800308	JP 1978-106541	19780830
	JP 62000905	B 19870110		
	EP 40896	A2 19811202	EP 1981-200767	19790820
	EP 40896	A3 19820203		
	EP 40896	B1 19840425		
	•	I, FR, GB, IT, NL,	SE	
PRAI	JP 1978-102614	A 19780822		
	JP 1978-106541	A 19780830		
	EP 1979-301696	A 19790820	`	
GI				

AB Amides I (R1, R2, R3, R4 = H, halo, OH, trihalomethyl, Ph, PhO, PhS, C1-6 alkyl, hydroxyalkyl, alkenyl, alkoxy, alkylthio, dialkylamino, alkylsulfonyl; R1R2 or R3R4 = ring; R3 = H or R1) were prepared by hydrolysis of the corresponding nitriles in presence of quaternary ammonium compds. and in aqueous alkaline H2O2. The amides I were converted to

corresponding amines by treatment with hypohalites. Thus, PhCH2CN with 4-MeC6H4CH4Cl gave PhCH(CN)CH2C6H4Me-4, which on hydrolysis in aqueous NaOH containing H2O2 and Bu4NOH gave PhCH(CONH2)CH2C6H4Me-4 (II). II in MeOH containing NaOH was treated with Br at 0° and a catalytic amount of Bu4NOH and the mixture refluxed to give PhCH2CH(NH2)CH2C6H4-Me.

IT 74533-40-7P 74533-41-8P 74533-42-9P

74533-47-4P 74533-54-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with hypohalite)

RN 74533-40-7 CAPLUS

CN Benzenepropanamide, 4-methyl $-\alpha$ -(4-methylphenyl)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{O} \\ \text{C-NH}_2 \\ \text{CH-CH}_2 \\ \text{Me} \end{array}$$

RN 74533-41-8 CAPLUS

CN Benzenepropanamide, α -(4-chlorophenyl)-4-methyl- (CA INDEX NAME)

RN 74533-42-9 CAPLUS

CN Benzenepropanamide, α -(3-bromophenyl)-4-methyl- (CA INDEX NAME)

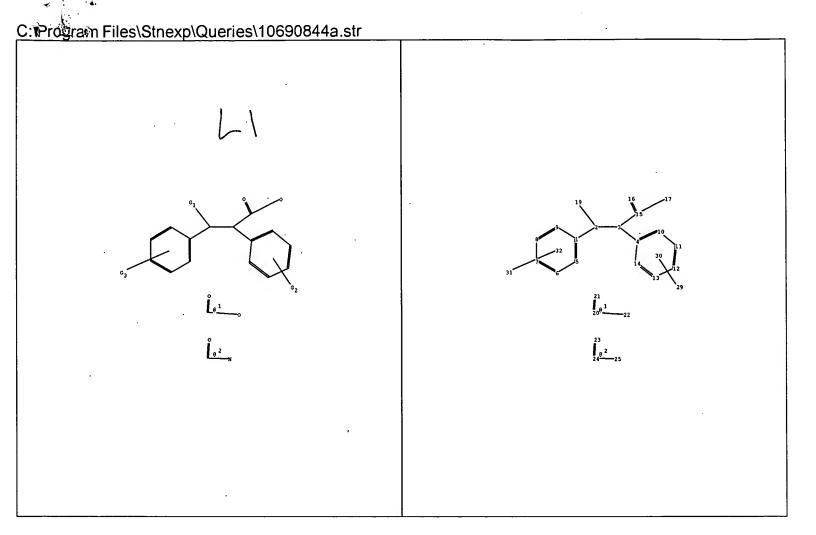
RN 74533-47-4 CAPLUS

CN Benzenepropanamide, α -(3-hydroxyphenyl)-4-propyl- (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \\ & & \\ & C-NH_2 \\ \hline & CH-CH_2 \\ \hline & \\ & Pr-n \end{array}$$

RN 74533-54-3 CAPLUS

CN Benzenepropanamide, 2-ethyl- α -(3-methylphenyl)- (CA INDEX NAME)



chain nodes:

2 3 15 16 17 19 20 21 22 23 24 25 29 31

ring nodes:

1 4 5 6 7 8 9 10 11 12 13 14

chain bonds:

1-2 2-3 2-19 3-4 3-15 15-16 15-17 20-21 20-22 23-24 24-25

ring bonds:

1-5 1-9 4-10 4-14 5-6 6-7 7-8 8-9 10-11 11-12 12-13 13-14

exact/norm bonds:

2-19 15-16 15-17 20-21 20-22 23-24 24-25

exact bonds:

1-2 2-3 3-4 3-15

normalized bonds:

1-5 1-9 4-10 4-14 5-6 6-7 7-8 8-9 10-11 11-12 12-13 13-14

G1:H,Ak,OH

G2:Ak,OH,SO2,NH,X,[*1],[*2]

G3:X,Ak,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,SO2,NH,[*1],[*2]

Connectivity:

₹3:3-E exact RC ring/chain

Match level:

1:Atom 2:CLASS3:CLASS4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS16:CLASS17:CLASS19:CLASS20:CLASS21:CLASS22:CLASS23:CLASS 24:CLASS25:CLASS29:CLASS30:Atom 31:CLASS32:Atom

=> d his

(FILE 'HOME' ENTERED AT 09:59:03 ON 27 DEC 2007)

FILE 'REGISTRY' ENTERED AT 10:00:33 ON 27 DEC 2007

L1 STRUCTURE UPLOADED

L2 12 S L1

L3 282 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:01:14 ON 27 DEC 2007

L4 146 S L3

=> d 11

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT * Structure attributes must be viewed using STN Express query preparation.

 \Rightarrow d bib abs hitstr 55-146

ANSWER 55 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1996:193712 CAPLUS 124:316690

L4 AN DN TI Synthesis of 1,3,6,8-tetramethoxy-cis-4b,5,9b,10-tetrahydroindeno[2,1-

ajindene-5, 10-dione
Bianchi, D. E.; Alesso, E. N.; Iglesias, G. Y. Moltrasio
Departamento Quimica Organica, Universidad Buenos Aires Junin 956 (1113),
Buenos Aires, Argent. Organic Preparations and Procedures International (1996), 28(2), 230-4 CODEN: OPPIAK: ISSN: 0030-4948 Organic Preparations and Procedures, Inc. Journal so

English CASREACT 124:316690

The title compound I was prepared in 5 steps from (3,5-dimethoxyphenyl) acetonitrile. I will be used in an investigation of the synthesis of pallidol.
176386-39-39 176386-40-6p
RL: RCT (Reactant): 5FN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation of tetramethoxyindenoindenedione)
176386-39-3 CAPUS
Butanedioic acid, 2,3-bis(4-hydroxyphenyl)-, diethyl ester, (R*,R*)- (9CI)
(CA INDEX NAME)

Relative stereochemistry

176386-40-6 CAPLUS Butamedioic acid, 2,3-bis(4-hydroxyphenyl)-, diethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

ANSWER 56 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1995;402285 CAPLUS 122:290768
Some reactions of (3,4,5-trimethoxybenzylidene)-4-methoxyacetophenone Mahnoud, M. R.; Ebrahim, Avatef E. F.; Abd-El-Halim, M. S.; Radwan, A. M. Faculty Science, Ain Shams University, Cairo, Egypt Indian Journal of Heterocyclic Chemistry (1994), 4(2), 131-6 CODEN: IJCHEI; ISSN: 0971-1627 Journal English
Some new pyrazolines have been prepared by the reaction of (3,4,5-trimethoxybenzylidene)-4-methoxyacetophenone (1) with hydrazines in different media. Unexpected bromination is observed on treatment of 1 with bromine to give the pentabromo derivative, which was reacted with hydrazine hydrate and hydroxylamine hydrochloride. The behavior of 1 towards Et phenylacetate, Et cyanoacetate, and di-Et homophthalate under Michael conditions has also been studied. Reaction of 1 with thioglycollic and thiobarbituric acids have also been studied. 163074-91-5P
RL: SPN (Synthetic preparation); PREP (Preparation) (reactions of (trimethoxybenzylidene)methoxyacetophenone) 163074-91-5 CAPLUS Benzenepentanoic acid, a-[2-(ethoxycarbonyl)phenyl]-4-methoxy-6-oxo-β-(3,4,5-trimethoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 55 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN Relative stereochemistry. (Continued)

L4 AN DN TI

so

ANSWER 57 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1995;363883 CAPLUS 122:329535 Differentiation of meso- and dl-α-polysubstituted dibenzyl compounds by IR spectroscopy Zhang, Bin; Jia, Zhishing; Qi, Chenze Department of Chemistry, Lanchou University, Lanzhou, 730000, Peop. Rep. China Lanzhou Daxue Xuebao, Ziran Kexueban (1994), 30(1), 68-71 CODEN: LCTHAF; ISSN: 0455-2059 Lanzhou Daxue Journal Chinese Neso- and dl-diethyl-2,3-dicyano-2,3-di(p-X substituted phenyl) succinates (X = OMe, CH3, H, Cl, NO2) were studied by IR spectroscopy. The vibration wavenumbers of meso-isomers are higher at vc=o and lower at vc=o-c than those of the corresponding dl-isomers. 139257-67-3 139257-68-4 139257-70-8, meso-Diethyl-2,3-dicyano-2,3-di(p-chlorophenyl) succinate 139257-10-19tte); PRP (Properties): ANST (Analytical study) (differentiation of meso- and dl-α-polysubstituted dibenzyl compds. by IR spectroscopy)
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (2R,35)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

4 139257-68-4 CAPLUS
Butanediolc acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (ZR,SR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,35)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 57 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

139257-71-9 CAPLUS Butamedicia caid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR, JR)-rel- (9C1) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 58 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 58 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1994:680346 CAPLUS 121:280346

L4 AN DN TI

121:280346
Mass spectra of dL-diethyl 2,3-dicyano-2,3-bis(p-substituted phenyl)succinates
Li, Haiquan: Qi, Chenze: Zai, Jianjun: Zhao, Fanzhi: Chen, Nenyu: Hao, Xiumei: Yang, Dilun
Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China
Lanzhou Daxue Xuebao, Ziran Kexueban (1993), 29(3), 142-4
CODEN: LCTHAF: ISSN: 0455-2059 AU

The mass spectral of title compds. I (X = H, Cl, Me, MeO, NO2) were studied by means of low resolution EIMS and high resolution accuracy mass measuring MS. The fragmentation mechanism of the di-Et esters and structures of characteristic ions formed were discussed.

139257-68-4 139257-71-9

RL: PRP (Properties)
[mass spectra of di-Et dicyano(diphenyl) succinates)
139257-68-4 CAPLUS

Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (2R,3R)-rel- (9C1) (CA INDEX NAME)

Relative stereochemistry.

139257-71-9 CAPLUS Butanedicic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSVER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1994:500056 CAPLUS
121:100056
Bivalent ligands as probes of estrogen receptor action
Bergmann, Kathryn E.; Wooge, Cynthia H.; Carlson, Kathryn E.;
Katzenellenbogen, Benita S.; Katzenellenbogen, John A.
Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA
JOURNAL of Steroid Biochemistry and Molecular Biology (1994), 49(2-3),
139-52
CODEN: JSBBEZ; ISSN: 0960-0760
JOURNAL
English

The estrogen receptor (ER) is a hormone-regulated transcription factor which is thought to bind to specific DNA sequences as a homodimer. To better understand structural requirements for dimerization and its functional role in ER action, the authors synthesized a series of bivalent ligands based on the non-steroidal estrogen hexestrol (I). These mol. probes join two hexestrol mols. of the erythro (E. active) configuration with either 4 or 8 carbon linkers (II) (designated E-4-E (X = (CH2)4) and E-8-E (X = (CH2)8) series, resp.], or with longer linkers comprised of ethylene glycol units II (E-eg-E (X = CH2(H2OCH2)nCH2, n = 1-4) series). Several other bi- and monovalent control compds. were prepared The bivalent ligands bind to ER with a relative affinity I-7 that the estradiol. While most of the ligands demonstrated normal monophasic displacement curves in competitive binding assays with [3H] estradiol, uncharacteristic biphasic competitive binding curves were seen for some of the ligands, indicating possible structure-specific, neg. site-site interaction. In ER-deficient Chinese hamster ovary (CHO) cells transfected with an expression vector encoding ER, one series of bivalent ligands (E-4-E) had little stimulatory activity and inhibited transcription stimulated by hexestrol, as determined by a transient transfection assay using an estrogen-response reporter gene construct ((ERE)-TAH7-CAT, containing two estrogen response elements linked to a TATA promoter and the chloramphenical acetyl transferase reporter gene). Monovalent or control bivalent ligands failed to antagonize hexestrol-stimulated activity and were as fully active as hexestrol itself. Studies performed in MCF-7 human breast cancer cells, which contain endogenous ER, yielded similar bioactivity profiles for the E-4-E bivalent inhibitory ligands, showing them to be effective estrogen antagonists, when using either induction of

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) progesterone receptor or (ERE)2-TATA-CAT transcriptional activation as the endpoint. The E-8-E ligand, however, acted as partial agonist/antagonist of ERE-reporter gene transactivation and a full agonist of progesterone receptor induction in MCF-7 cells, thus showing cell- and response-specific differences in the effects of this bivalent ligand. These bivalent ligands for ER do not show enhanced potency or receptor binding affinity: however, some of them display binding properties that suggest the possibility of structure-specific neg. site-site interaction, and some of them function as quite effective estrogen antagonists. 156926-22-6 156926-24-8
RI: BIOL (Biological study)
(estrogen receptor binding by, antagonist activity in relation to) 156926-22-6 CAPLUS
Benzenepropanoic actid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-, 1,4-butanediyl ester, [αR*(α'R*,β'S*),βS*]-(-)-

Rotation (-). Absolute stereochemistry unknown.

156926-24-8 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -{4-hydroxyphenyl}-, 1,4-butanediyl ester, [α R*(α 'R*, β 'S*), β S*)- {9CI} (CA INDEX NAME)

Relative stereochemistry.

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

156840-31-2 156840-32-3 156840-33-4
156840-34-5 156840-35-6 156840-36-7
156840-37-8 156840-38-9 156840-39-0
RL: BIOL (Biological study)
(estrogen receptor binding by, bivalent analogs in relation to)
156840-31-2 CAPLUS
Benzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-,
ethyl ester, (R*,5*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-32-3 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -{4-hydroxyphenyl}-, butyl ester, (R*,5*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-33-4 CAPLUS
Benzenepropanoic acid, B-ethyl-4-hydroxy-a-(4-hydroxyphenyl)-,
octyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

156840-42-5 156926-25-9 RL: BIOL (Biological study) (estrogen receptor binding by, biol. activity in relation to) 156840-42-5 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, 1,8-octanediyl ester, [aR*(a'R*, β 'S*), β S*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156926-25-9 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, 1,8-octanediyl ester, [aR*(a'S*, β 'R*), β R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

HO O (CH₂)
$$\tilde{\gamma}^{\text{Me}}$$

156940-34-5 CAPLUS Benzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-, 4-hydroxybutyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-35-6 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, θ -hydroxyoctyl ester, (R^*, S^*) - [9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-36-7 CAPLUS
Benzenepropanoic acid, B-ethyl-4-hydroxyy-a-(4-hydroxyphenyl)-,
2-ethoxyethyl ester, [R*,5*]- [9CI] (CA INDEX NAME)

Relative stereochemistry.

RN 156840-37-8 CAPLUS

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Contine Benzenepropanoic acid, \$\textit{\textit{\textit{P}}-4-hydroxy-a-(4-hydroxyphenyl)-,}}{2-(2-ethoxyethoxy)ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-38-9 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, 2-(2-hydroxyethoxy)ethyl ester, (R^*, S^*) - (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-39-0 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -{4-hydroxyphenyl}-, 2-[2-(2-hydroxyethoxy)ethoxy]ethyl ester, (R^*, S^*) - (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-29-8 156840-30-1 156840-40-3
156840-41-4 156840-47-0 156840-48-1
156840-49-2 156840-50-5 156926-23-7
156926-28-2 156926-29-3 156926-30-6
156926-31-7
RL: BIOL (Biological study)
(estrogen receptor binding by, structure in relation to)
156840-29-8 CAPLUS
Benzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-,

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

156040-41-4 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, 1,3-propanediyl ester, [α R'(α 'R', β 'S'), β S')- (9CI) (CA INDEX NAME)

Relative stereochemistry.

156840-47-0 CAPLUS
Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, oxydi-2,1-ethanediyl ester, [α R*(α 'R*, β 'S*), β S*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME) (Continued)

Relative stereochemistry.

156840-30-1 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, 1,4-butanedyl ester, [α R*(α 'R*, β 'S*), β S*)-(+)-(9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

156840-40-3 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, l,2-ethanediyl ester, [aR*(a'R*,\beta'S*),\betaS*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

156940-48-1 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl}-, l,2-ethanediylbis(oxy-2,1-ethanediyl) ester, [α R*, α Y*, β S*), β S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-B

156840-49-2 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, oxybis(2,1-ethanediyl)-, ester, [α R', α 'R', β 'S'), β S')- [9CI). (CA INDEX NAME)

Relative stereochemistry.

(Continued)

PAGE 1-B

156840-50-5 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, 3,6,9,12-tetraoxatetradecane-1,14-diyl ester, [α R*(α 'R*, β 'S*), β S*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN oxydi-2,1-ethanediyl ester, [αR*(α'5*,β'R*),βR*]-(9CI) (CA INDEX NAME) (Continued)

Relative stereochemistry.

156926-29-3 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, 1,2-ethanedlylbis (oxy-2,1-ethanedlyl) ester, [aR*(α 'S*, β 'R*), β R*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-B

156926-30-6 CAPLUS
Benzenepropanoic acid, β-ethyl-4-bydroxy-e-(4-bydroxyphenyl)-,
oxybis(2.1-ethanoiyloxy-2,1-ethanodiyl) ester,
[aR*(a'5*,β'R*),βR*]- (9CI) (CA INDEX NAME)

L4 ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)

PAGE 1-A

PAGE 1-B

156926-23-7 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, 1.4-butanediyl ester, [α R'(α 'S', β 'R'), β R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 156926-28-2 CAPLUS CN Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-,

L4 ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN Relative stereochemistry. (Continued)

PAGE 1-A

PAGE 1-B

156926-31-7 CAPLUS

Benzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-,
3,6,9,12-tetraoxatetradecane-1,14-diyl ester,
[aN'(α'5*,β'N'),βN']- [9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

L4 ANSWER 59 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) PAGE 1-B

ANSWER 61 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1994:269805 CAPLUS 120:269805

120:269805 Scope and mechanism of the reaction of alkylidenephosphoranes with 10-methyleneanthrone Ganoub, Neven A. F.; Abdou, Wafaa M.; Yakout, El Sayed M. A. Dep. Pestic. Chem., Natl. Res. Cent., Cairo, Egypt Phosphorus, Sulfur and Silicon and the Related Elements (1993), 84(1-4), 197-204 CODEN: PSSLEC: ISSN: 1042-6507

Journal English

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Quinone methide I reacts with excess (carbomethoxymethylene)triphenylphosphorane to afford bisanthracenol II (R - COZMe), III (RI - Me), and ylides IV and V; reaction of I with (carbethoxymethylene)triphenylphosphorane gave similar and different products. The polarity of the solvent had a limited effect on the reaction. Mechanistic studies suggest that I can react as a Diels-Alder diene and function as a dienophile in the same reaction. Wittig reactions of IV and V with BzH were described.

RISPN (Synthetic preparation): PREP (Preparation) (preparation and Wittig reaction with benzaldehyde)

154504-11-7 CAPLUS

9-Anthracenepropanoic acid, 10-[1-[(10-hydroxy-9-anthracenyl)methyl]-2-methoxy-2-oxocthyl]-a-(triphenylphosphoranylidene)-, methyl ester (9CI) (CA INDEX NAME)

154504-14-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
154504-14-0 CAPUS
9-Anthracenepropanoic acid, 10-[1-[(10-hydroxy-9-anthraceny1)methy1]-2-methoxy-2-oxocethy1]-a-(pheny1methy1ene)-, methy1 ester (9CI) (CA
INDEX NAME)

ANSWER 60 OF 146 CAPLUS COPYRIGHT 2007 ACS ON STN 1994:270919 CAPLUS 120:270919

120:270919
Synthesis of saulatine
Kim, Dong Chin; Yoon, Won Hyung; Choi, Hoon; Kim, Dong H.
Dep. Chem., Pohang Inst. Sci. Technol., Pohang, 790-600, S. Korea
Journal of Heterocyclic Chemistry (1993), 30(5), 1431-6
CODEN: JHTCAD: ISSN: 0022-152X

Journal English CASREACT 120:270919

A study directed toward the synthesis of saulatine (5,8,9,14a-tetrahydro-3,4,11,12-tetramethoxyisoquino[1,2-b]benzazepine-6,14-dione) (I) is described. The successful synthetic route consists of three steps starting with 3,4-dimethoxyphenethylamine and 2-bromo-(3,4-dimethoxy-2-ethoxycarbomethylphenyl) acetate. The methoxy moieties present on the aromatic rings prohibit the use of the intramol. Friedel-Crafts reaction

ΙT

a Lewis acid catalyst for ring construction because of their demethylation tendency under the reaction conditions.
154534-99-3P
RL: PREP (Preparation)
(intermediate in attempted synthesis of saulatine)
154534-99-3 CAPUNS
Butanedioic acid, 2,3-bis(2-bromo-4,5-dimethoxyphenyl)-, diethyl ester
(9CI) (CA INDEX NAME)

ANSWER 61 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4	ANSWER 62 OF 146 C	APLUS	COPYRIGHT 2	007 ACS on STN	
AN	1994:163733 CAPLUS				
DN	120:163733				
TI	Hydrazone derivativ active ingredient a	e insec	ticides and	or acaricides contain mpounds thereof	ing the same
IN				, Shigeru: Isayama, Sh	inji
PA					-
50					
DT					
LA					
FAN.	CNT 1			ADDITIONATION NO	
	PATENT NO.		DATE	APPLICATION NO.	
PΙ		A2		EP 1993-106584	19930422
		A3			
	R: CH, DE, ES,				
	CA 2094333	A1	19931024	CA 1993-2094333	19930419
	US 5451607	A	19950919	US 1993-47490	19930419
	JP 06056754	A	19940301	JP 1993-94674	19930421
	BR 9301628	A	19931026	BR 1993-1628	19930422
	AU 9337063	A	19931028	AU 1993-37063	19930422
	AU 657215		19950302		
PRAT	JP 1992-131616	A	19920423		
os	MARPAT 120:163733	••			
GI			•		

The title compds. I [A = (CH2)t, O, S(O)n, OCH2, (un)substituted NH, etc.; n = 0-2; t = 1-3; Rl = halogen, CN, MO2, azide, etc.; R2 = H, Cl-6 alkyl, Cl-6 haloalkyl, C3-6 cycloalkyl, C2-6 alkenyl, (un)substituted Ph, etc.; R3 = H, Cl-6 alkyl, Cl-6 haloalkyl, C2-6 alkenyl, C2-6 haloalkenyl, C2-6 alkynyl, etc.; R4 = H, Cl-6 alkyl, Cl-6 haloalkyl; R5 = Cl-6 alkyl, Cl-6 haloalkyl; C2-6 alkenyl, C2-6 alkenyl, C2-6 alkyl, Cl-6 haloalkyl; R5 = Cl-6 alkyl, Cl-6 haloalkyl; C2-6 alkyl, C2-6 alkenyl, C2-6 alkylyl, etc.; R6 = H, Cl-6 alkyl, C2-6 alkenyl, C2-6 alkenyl, C2-6 alkylyl, etc.; R6 = H, Cl-6 alkyl, C2-6 alkenyl, C2-6 alkenyl, C2-6 alkynyl, etc.; R6 = H, Cl-6 alkyl, C2-6 alkenyl, C2-6 alkenyl, C2-6 alkynyl, etc.; R6 = H, Cl-6 alkyl, C2-6 alkenyl, C2-6 alkenyl, C2-6 alkynyl, etc.; R6 = H, Cl-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, etc.; R6 = H, Cl-6 alkyl, C2-6 alkyl, C2-6 alkynyl, etc.; R6 = H, Cl-6 alkyl, C2-6 a

			•			
L4	ANSWER 63 OF 146 CAN	PLUS COPYRIGHT	2007 ACS on STN			
AN						
DN	120:134276					
TI	Agrochemical arthropo	odicidal amides				
IN	Amoo, Victor Ekow: At	nnis, Gary David	d; March, Robert William	ı, Jr.		
PA	du Pont de Nemours, I	E. I., and Co.,	USA			
50	PCT Int. Appl., 129	pp.				
	CODEN: PIXXD2	•				
DT	Patent					
LA	English					
FAN.	.CNT 1					
	PATENT NO.	KIND DATE	APPLICATION NO.	DATE		
PI			WO 1993-US2434			
			JP, KP, KR, KZ, LK, MG,	MN, MW, NO,		
		RU, SD, SK, UA,				
			GB, GR, IE, IT, LU, MC,			
			GN, ML, MR, SN, TD, TG			
	AU 9338118	A 19931021	AU 1993-38118	19930318		
	EP 632803	Al 19950111	EP 1993-907555	19930318		
		B1 19981209				
	R: ES, FR, IT					
	JP 07507276	T 19950810		19930318		
	JP 3446052	B2 20030916				
	BR 9306225 ES 2127270	A 19980630		19930318		
	ES 2127270	T3 19990416	ES 1993-907555	19930318		
	CN 1098093					
	US 5514678	A 19960507		19940922		
PRA	I US 1992-858205					
	US 1992-875174	A2 19920428				
	WO 1993-US2434	A 19930318				
os	MARPAT 120:134276					
GI						

ANSWER 62 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
153278-90-1P
RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, in preparation of hydrazone insecticides)
153278-90-1 CAPLUS
Benzenepropanoic acid, 3-chloro-\alpha-(4-chlorophenyl)-, ethyl ester
(CA INDEX NAME)

ANSWER 63 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSVER 64 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1993:494855 CAPLUS 119:94855 Laser Raman spectroscopic study on two isomers of a-polysubstituted dibenzyl compounds Qi, Chenze: Zhang, Din; Jia, Xueqing; Yang, Dilun Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China Guangpuxue Yu Guangpu Fenxi (1992), 12(4), 11-14 CODEN: GYCFED: ISSN: 1000-0593

Oddanjpusus to Joseph 1000-0593
Journal
Chinese
Five pairs of meso- and dL-4-XCGH4C(CN) (CO2Et)C(CN) (CO2Et)CGH4X-4 (X = H, Cl, He, MeO, NO2) have been studied by laser Raman spectroscopy. The
Raman bands of some groups have been analyzed. The effect of different
configurations on the laser Raman spectra is discussed.
139257-67-3 139257-68-4 139257-70-8
139257-71-9
RL: PRP (Properties)
(Raman spectrum of)
139257-67-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester,
(2R,35)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-68-4 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester,
(2R,3R)-rel- (9CI) (CA INDEX NAME)

139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (2R,35)-rel- (9CI) (CA INDEX NAME)

ANSWER 65 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1993:491499 CAPLUS 119:91499 CAPLUS 119:91499 Effect of molecular configuration and substituent electronic effect on carbon-13 NMR spectra of diethyl 2,3-dicyano-2,3-bis(p-substituted phenyl)succinates Yang, Dilun: Qi, Chenze Wu, Jingjiar Cui, Yuxinz Liu, Youcheng Dep. Chem. Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China Gaodeng Xuexiao Huaxue Xuebao (1993), 14(2), 257-60 CODEN: KTHPDM; ISSN: 0251-0790 Journal Chinese

$$x - \begin{cases} cN & cN \\ c & c \\ cO_2Et & cO_2Et \end{cases} - X$$

The meso (I: X = OCH3, CH3, H, Cl, NO2) and dL isomers (II: same X) of the title esters are studied by 13C NMR spectrometry. The chemical shifts of

carbon atoms in the same group on both sides of the central C-C bond are equivalent, and the chemical shifts of the C7-C9 atoms in II are smaller than in

In I. Plots of chemical shifts of C6, C7 and C8 atoms vs. Hammett o consts. of substituents in the para position of the benzene ring are

Relative stereochemistry.

139257-68-4 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester,

L4 ANSWER 64 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 65 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (2R, 3R) -rel- (9CI) (CA INDEX NAME) (Continued)

Relative stereochemistry.

139257-70-8 CAPLUS Butanedicic acid, 2, 3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (2R,35)-rel- (9Cl) (CA INDEX NAME)

Relative stereochemistry.

139257-71-9 CAPLUS Butanedioic acid. 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester. (ZR,JR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 66 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1993:408231 CAPLUS 119:8231

119:8231
Study on the mechanism of oxidative coupling reactions of ethyl a-cyano-p-X-substituted phenylacetates by using the catalyst [Cu2* (OH-)TMED) 2C12
Yang, Dilun: Qi. Chenze: Lu, Minglan: Liu, Youcheng
Dep. Chem., Lanzhou Univ., 730000, Peop. Rep. China
Huaxue Xuebao (1993), 51(1), 66-72
CODEN: HHHPA4: ISSN: 0567-7351

DT LA GI

£ì.

The oxidative coupling reactions of the title compds. I (X = OCH3, CH3, H, Cl, NO2) with Cu2+-TMEDA-O2 (TMEDA = N,N,N',N'-tetramethylenediamine) system give meso- and dl-succinates II. On the basis of the stereochem. and IR, IH NMR and EPR determination of the reactive intermediates of the oxidative coupling reactions, the mechanism was suggested.

139257-61-3P 139257-68-4P 139257-70-8P

139257-71-9P
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of)
139257-67-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester,
(ZR,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-68-4 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (ZR,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 67 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1993:256345 CAPLUS .

DN 118:256345 .

I Manufacture of fiber-reinforced plastic products and prepregs
IN Araki, Shigeo
RA Kaysku Noury Corp, Japan
SO Jph. Kokai Tokkyo Koho, 6 pp.
CODEN: JKCKAF

DT Patent
LA Japanese
FANLCNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE PI JP 05009246 A 19930119 JP 1991-160844 19910606
PRAI JP 1991-160844 19910606
AB The title products are manufactured by curing prepreg materials containing

The title products are manufactured by curing prepreg materials containing and, polyesters or vinyl ester resins in the presence of R3C6H4CRIRZCRIRZCGH4R3 (R1 = cyano, CO2Me, CO2Et: R2 = CO2Me, CO2Et: R3 = H, Me, OMe) at 60-100°. Thus, a glass mat was was impregnated with a composition containing Polylite 8010 100, NS 100 100, 1,2-bis(p-methoxyphenyl)-1,2-dicarboethoxy-1,2-dicyanoethane 1, Zn stearate 4, and Mg0 0.5 part, sandwiched between polyethylene films, and kept at 20° for 7 days to give a prepreg mat showing gelation time >180 days at 20° and giving cured product with Barcoll hardness 60.

31249-03-3 34404-72-3, 1,2-Bis(p-methylphenyl) tertacarboenthoxyethane 70230-43-2
147992-58-3 147992-59-4 147992-60-7,
1,2-Bis(p-methylphenyl) tetracarboethoxyethane
RL: CAT (Catalyst use): USES (Uses)
(catalysts, unsatd. polyesters and vinyl ester resins containing, for prepregs with long shelf life)
31249-03-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester (9C1) (CA INDEX NAME)

34404-72-3 CAPLUS
1,1,2,2-Ethanetteracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetramethyl ester (9CI) (CA INDEX NAME)

ANSWER 66 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,35)-cel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,3R)-rel (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 67 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

70230-43-2 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, 1,4-diethyl ester (CA INDEX NAME)

147992-58-3 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2,4-dimethylphenyl)-, diethyl ester (9C1) (CA INDEX NAME)

147992-59-4 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2,4-dimethylphenyl)-, dimethyl ester (9C1) (CA INDEX NAME)

147992-60-7 CAPLUS 1.1.2,2-Ethanetetracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetraethyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 67 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

$$\mathsf{Me} = \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\mathsf{Eto-C}} \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\mathsf{Ne}} \mathsf{Me}$$

4

L4 ANSWER 68 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,35)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-71-9 CAPLUS Butamedicic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 68 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1993:22683 CAPLUS 118:22683 CAPLUS 118:22683 Synthesis of diethyl 2,3-dicyano-2,3-bi(p-substituted phenyl)succinates and its decomposition in styrene Yang, Dilun; Qi, Chenzer Li, Zhaolong; Liu, Youcheng Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China Gaodeng Xuexiao Huaxue Xuebao (1991), 12(12), 1623-6 CODEN: RTHPON: ISSN: 0251-0790 Journal Chinese CASREACT 118:22683 Di-Et 2,3-dicyano-2,3-bis(p-X-phenyl)succinates (X - MeO, Me, Cl, NO2) were prepared by oxidative coupling of the corresponding Et (cyanophenyl)acetates, and their meso and dl isomers were separated and characterized by proton NMR, IR, x-ray, and mass spectroscopy. The thermal decomposition rates of the meso-isomers of these succinates in

DT LA OS AB

styrene
at 100° were greater than those of the dl-isomers except for the
isomer with X = MeO. The substituent effect on the thermal decomposition

of these succinates followed the order: MeO > Me > Cl > H.

139257-67-3P 139257-68-4P 139257-70-8P

139257-17-9P

RL: RCT (Reactant): PREF (Preparation): RACT (Reactant or reagent)
(synthesis and decomposition of)

139257-67-3 CAPLUS

Butanedioic acid, 2, 3-dicyano-2, 3-bis(4-methylphenyl)-, diethyl ester,
(2R,35)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-68-4 CAPLUS Butamedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (ZR,R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 69 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1993:21868 CAPLUS 118:21868

L4 AN DN TI

118:21868
Studies on the proton NMR spectra of meso and dl diethyl
2,3-dicyano-2,3-bis(p-substituted phenyl)succinates
Yang, Dilun; Qi, Chenzer Cui, Yuxin; Dang, Haishan; Liu, Youcheng
Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China
Gaodeng Xuexiao Huaxue Xuebao (1991), 12(12), 1627-30
CODEN: KTHEPM: 15SN: 0251-0790 AU CS SO

DT LA AB Journal Chinese

The IH NMR of meso- and d1-diethyl 2,3-dicyano-2,3-di(p-X-phenyl) succinates (X = OCH3, CH3, H, Cl, NO2) and IH Noesy spectra of meso- and d1-isomers of the di-Et ester with X = CH3 were determined by using a

di-isomers of the di-Et ester with X = CH3 were determined by using a Bruker AM

400 MHz superconducting NMR spectrometer. The corresponding proton of the substituent groups attached to the two central C atoms in the mols. are chemical shift equivalence. The average difference between o-IH absorptions of

Ph in the dl-isomers and that in meso-isomers was found to be .hivin.A5dl-meso = -120.1 ± 6.1 Hz. All of the meso-isomers, then, have methylene (ABX3 system) and Me in the ethoxy at upfield positions, and all of the dl-isomers have that at downfield positions. hivin.A5dl-meso = 53.3 ± 5.9 Hz and .hivin.A5dl-meso = 53.5 ± 5.9 Hz and .hivin.A5dl-meso = 53.5 ± 5.9 Hz and .hivin.A5dl-meso = 53.5 ± 5.8 Hz for protons in the methylenes, and .hivin.DVdl-meso = 39.3 ± 3.5 Hz for protons in the methyls. .hivin.A5dl-meso Is the mark of influence of mol. configuration on the chemical shift.

IT 139257-67-3 139257-68-4 139257-70-8

139257-71-9

RL: PRP (Properties)

13925/-71-9
(proton NMR of, mohoequivalents of methylene group in)
139257-67-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester,
(2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-68-4 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (ZR,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 69 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

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139257-70-8 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (2R,35)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

139257-71-9 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (ZR,JR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 70 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

144633-01-2 CAPLUS Butanedicic acid, 2,3-bis[3,5-bis[trifluoromethyl]phenyl]-, diethyl ester, [R*,5*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

144633-02-3 CAPLUS Butanedioic acid, 2,3-bis[4-(trifluoromethyl)phenyl]-, diethyl ester, (RY.51)- (9C1) (CA INDEX NAME)

Relative stereochemistry.

144633-04-5 CAPLUS Butanedioic acid, 2,3-bis[2-(trifluoromethyl)phenyl]-, diethyl ester, (R^*,R^*) - (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 70 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1992:651025 CAPLUS 117:251025 Electrochemistry of ethyl a-bromo-a-fluoro(phenyl)acetate and some ethyl a-bromo(trifluoromethylphenyl)acetates and electrochemical synthesis of the corresponding diastereoisometic diethyl succinates

Succinates and the control of the corresponding disastered: Matthello, Leonardo, Rampazzo, Liliana; Sotgiu, Giovanni Dip. IOMHM, Univ. Roma 'La Sapienza', Rome, ODI61, Italy Journal of Chemical Research, Synopses (1992), (10), 321 CODEN: JRFSDC: ISSN: 0308-2342

Electrolysis of PhCFBrCO2Et and title bromo(trifluoromethyl)phenylacetates I (R1 = CF3, R2-R4 = H: R1 = R3 = R4 = H, R2 = CF3, R1 = R3 = H, R2 = R4 = CF3) nn reticulated vitreous carbon in DMF gave disers PhCF(COZET)CF(COZET)Ph and II. II were obtained as mixture of meso- and DL-forms. 144633-09-5P 144633-00-1P 144633-01-2P 144633-07-8P 144633-07-8P RL: SFN (Synthetic preparation); PREP (Preparation) (preparation of) 144632-99-5 CAPLUS Butanedioic acid, 2,3-bis[2-(trifluoromethyl)phenyl]-, diethyl ester, (R*,5*)- (SCI) (CA INDEX NAME)

Relative stereochemistry.

144633-00-1 CAPLUS Butanedioic acid, 2,3-bis[3-(trifluoromethyl)phenyl]-, diethyl ester, (%,5:)- (9C1) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 70 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

144633-05-6 CAPLUS Butanedioic acid, 2,3-bis[3-(trifluoromethyl)phenyl]-, diethyl ester, (%*,8*)- (9C1) (CA INDEX NAME)

Relative stereochemistry.

144633-06-7 CAPLUS Butanedioic acid, 2,3-bis(3,5-bis(trifluoromethyl)phenyl]-, diethyl ester, (R^{*},R^{*})- (9CI) (CA INDEX NAME)

Relative stereochemistry.

144633-07-8 CAPLUS

Butanedioic acid, 2,3-bis[4-(trifluoromethyl)phenyl}-, diethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 70 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 71 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (halo)alkynyl, G3-6 (halo)cycloalkyl, halo, cyano, N3, etc. or R2R2 = OCH2O, OCF2O, OCH2CH2O, etc.; R3 = H, N3, N02, halo, C1-6 (halo) alkyl, C2-6 alkenyl, (substituted) Ph, etc.; R4, R5 = H, C1-4 alkyl, etc.; R4R5 = O, S; R8 = (substituted) Ph, etc.; R4, R5 = H, C1-4 alkyl, C2-4 (halo)alkenyl, (substituted) Ph, -pyridyl or R8R9 = (CH2)4, (CH2)5, etc.; R31 = H, C1-4 alkyl, C2-4 alkonycarbonyl, (substituted) Ph, -pyridyl or R8R9 = (CH2)4, (CH2)5, etc.; R31 = H, C1-4 alkyl, C2-4 alkanycarbonyl) etc. Physical Phys

L4	ANSWER 71 OF 146 C	APLUS COPYRIGHT	2007 ACS on STN			
AN	1992:634026 CAPLUS					
DN	117:234026					
TI	Preparation of inde	nooxadiazinecarb	oxamides as arthropodicie	des		
IN			m Eldo; McCann, Stephen			
	Wing, Keith Dumont					
PA	du Pont de Nemours,	E. I., and Co.,	USA			
50	PCT Int. Appl., 351		•			
	CODEN: PIXXD2	rr.				
DT	Patent					
LA	English					
	CNT 1					
	PATENT NO.	KIND DATE	APPLICATION NO	DATE		
			APPLICATION NO.			
PI	WO 9211249 *	A1 19920709	WO 1991-US9164			
			HU, JP, KP, KR, LK, MG,			
	PL, RO, SD,		110, 01, 111, 111, 111, 110,	,,,		
			CI, CM, DE, DK, ES, FR,	GA GR GN		
		MC, ML, MR, NL,		011, 02, 011		
	CA 2098612	A1 19920622	CA 1991-2098612	19911217		
	C) 2000C12	C 20020507		.,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		
	AU 9191270	A 19920722	AU 1991-91270	19911217		
	AU 659121	B2 19950511				
	AU 659121 EP 565574	A1 19931020		19911217		
	EP 565574	B1 19950802		.,,,,,,,,,		
	R: AT. BE. CH.		GB, GR, IT, LI, LU, MC,	NL. SE		
	HU 65223	A2 19940502		19911217		
	HU 213635	B 19970828				
	HU 65223 HU 213635 JP 06504777 BR 9107246 ES 2077392	T 19940602		19911217		
	BR 9107246	A 19940614	BR 1991-7246	19911217		
	ES 2077392	T3 19951116	ES 1992-902235	19911217		
	RU 2096409 ZA 9110002	C1 19971120	RU 1991-5011055	19911217		
	ZA 9110002	C1 19971120 A 19930621	ZA 1991-10002	19911219		
	ZA 9110002 IL 100429 CN 1062726 CN 1034468 US 5462938 US 5708170	A 19960119	RU 1991-5011055 ZA 1991-10002 IL 1991-100429	19911219		
	CN 1062726	A 19920715	CN 1991-111730	19911221		
	CN 1034468	B 19970409				
	US 5462938	A 19951031	US 1993-75534	19930618		
	US 5708170 US 1990-632438	A 19980113		19950523		
PRAI	US 1990-632438	A2 19901221				
	US 1991-714401	A2 19910611 A 19911217				
	WO 1991-US9164	A 19911217	•			
	US 1993-75534	A3 19930618				
os	CASREACT 117:234026	: MARPAT 117:234	026			

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Title compds. QC(:X)NYG and QXIC:NG [I and II; Q = Q1, Q2, etc.; A = H; E = H, C1-3 alkyl or AE = CH2, CH2CH2, O, S, SO, SO2, OCH2, SCH2, etc.; G = (substituted) Ph, -pyridyl, -pyrimidyl, -thienyl, etc.; X = O, S, NX2; X1 = C1, Br, QR8, SR8, NR8R9; X2 = R8, OH, QR8, cyano, SOZR8, SOZPh, etc.; Y = H, C1-6 (halo)alkyl, CH2Ph, C2-6 alkoxyalkyl, C2-6 alkenyl, C2-6 alkynyl, C1-3 alkoxy, cyano, NO2, (substituted) Ph, etc.; Z = C, N; Z1 = O, S, NR31; R2 = H, (substituted) C1-6 alkyl, C2-6 (halo) alkenyl, C2-6

GI

ANSWER 72 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1992:625501
1992:625501
Identification of the configurations of dl and meso-diethyl 2,3-dicyano-2,3-diphenylsuccinates and its p-(X) -substituted phenyl derivatives (X=H, CH3, OCH3) by FAB-B/E link scan metastable ion spectrometry Li, Haiquan; Zhao, Fanzhi; Zai, Jianjun; Chen, Nengyu; Qi, Chenze; Yang, Dilun; Liu, Youcheng
Instrum. Anal. Res. Cent., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China
Gaodeng Xuexiao Huaxue Xuebao (1991), 12(11), 1540-1
CODEN: KTHPDH; ISSN: 0251-0790
Journal
Chinese
In this paper, three pairs of dl and meso-diethyl 2,3-dicyano-2,3-diphenylsuccinate and its derivs. of p-(X) substituted Ph succinates (X = H, CH3, OCH3) were analyzed by using FAB-B/E (magnetic field/static elec. field) linked scan metastable ion spectrometry. The effect and applicability of this method in identification of the configuration of these isomers are discussed.
139257-67-3 139257-68-4, dl-Diethyl 2,3-dicyano-2,3-di(p-methylphenyl) succinate and its derivs. PROC (Process)
(identification of, by FAB-B/E link scan metastable ion spectrometry)
139257-67-3 CAPLUS
BUtanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (2R,35)-rel- (SCI) (CA INDEX NAME)

Relative stereochemistry.

139257-68-4 CAPLUS Butamedioid acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (ZR,JR)-rel-(9CI) (CA INDEX NAME)

ANSWER 73 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1992:448048 CAPLUS
117:48048 CAPLUS
117:48048 CAPLUS
117:48048 CAPLUS
117:48048 CAPLUS
117:48048 CAPLUS
Reichir Nakajima, Shoichi
Fac. Pharm. Sci., Hoshi Univ., Tokyo, 142, Japan
Chemical & Pharmaceutical Bulletin (1992), 40(4), 1037-8
CODEN: CPBTAL: ISSN: 0009-2363
JOURNAL
LENGISH
CASREACT 117:48048
Electrochem. methoxylation at the active methylene group of phenylacetates
and 1-naphthaleneacetate was conducted successfully at room temperature in
methanol containing potassium iodide as electron carrier and sodium
looxide

methanol containing pota-sium iodide as electron carrier and sodium methoxide
as base and methoxylating agent. Along with the monomethoxylated products, dimethoxy, hydroxy, and oxo derivs. as well as the dimers (auccinates) were produced as byproducts.

1 142472-20-6F
RI: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in electrochem. methoxylation of Me arylacetate)
RN 142472-20-6 CAPLUS
CN Butanedioic acid, 2,3-bis(4-chlorophenyl)-, dimethyl ester (9CI) (CA INDEX NAME)

(Continued) ANSWER 74 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

CRN 139257-68-4 CMF C24 H24 N2 O4

Relative stereochemistry.

CM 2

CRN 56-23-5 CMF C C14

139257-70-8 CAPLUS

Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (2R,3S)-rel- (9CI) (CA INDEX NAME)

139257-71-9 CAPLUS

Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, diethyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

ANSVER 74 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1992:117741 CAPLUS 116:117741 CAPLUS 116:117741 CAPLUS 116:117741 CAPLUS 2,3-dicyano-2,3-dicyano-2,3-dicyano-2,3-dicyano-2,7

Chinese
The crystal and mol. structures of meso- and dl-diethyl
2,3-dicyano-2,3-di(p-X-substituted phenyl) succinates, X:OCH3, meso (1),
dl-1 (11): X = CH3 meso-(111):, dl-(1V):, X = Cl (V), meso-(VI), dl were
determined I decomposed when its diffraction at a were being collected.

monoclinic, space group P21/c; final R = 0.0413 for 2488 reflections. III is triclinic space group P.hivin.1; a = final R = 0.0501 for 2191 observed reflections. IV is triclinic, space group P.hivin.1; a = final R = 0.0804 for 3049 observed reflections. V is monoclinic, space group P21/c; a =

for 3049 observed reflections. V is monoclinic, space group P21/c: a = 1
R = 0.0585 for 1460 reflections. VI is monoclinic, space group P21/c: a = 1
final R = 0.0521 for 2347 reflections. Atomic coordinates are given. In comparison with normal C-C single bond (0.1544 mm), the bond length for the central C-C bond in all of the diastereciosmers shows a remarkable lengthening effect of 0.0023-0.0052 (nm) (1.4-3-4%). The bond length for the central bonds in all of meso-isomers is longer than that in corresponding dl-isomers. Among the substituted groups attached to the 2 central C atoms in the mols. of all of the diastereoisomers rep., the interat. distance between nonbonded atoms is smaller than the sum of Van der Waals radii, indicating the existence of serious steric hindrance which is mainly responsible for the lengthening effect.
139257-01-3 139257-69-5 139257-70-8
RI: PRP (Properties)

His PRP (Properties)
(crystal structure of)
19257-67-3 CAPLUS
Butanedioic acid, 2, 3-dicyano-2, 3-bis(4-methylphenyl)-, diethyl ester,
(ZR, 35)-rel- (9C1) (CA INDEX NAME)

Relative stereochemistry.

139257-69-5 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, diethyl ester, (R.R.)-, compd. with tetrachloromethane (1:2) (9C1) (CA INDEX NAME)

CM 1

ANSWER 74 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 75 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1991:206840 CAPLUS
114:206840
5ynthesis of 5'-[1-(methoxycarbonyl)-2-(p-methoxyphenyl)ethyl)- and
5'-(2-(methoxycarbonyl)-1-(p-methoxyphenyl)ethyl]-2',3',4,4',6'pentamethoxychalcone
Obara, Heitaro; Onodera, Junichi; Tsuchiya, Mitsuhiro; Matsuda, Hiroyuki;
Sato, Shingo; Matsuda, Shigeru
Fac, Eng., Yamagata Univ., Yonezawa, 992, Japan
Bulletin of the Chemical Society of Japan (1991), 64(1), 309-11
CODEN: BCSJ08; ISSN: 0009-2673
Journal
English
CASREACT 114:206840 L4 AN DN TI

Pentamethoxychalcone derivs. (E)-I [R = CO2Me, Rl = p-MeOCGH4CH2 and R = CH2CO2Me, Rl = p-MeOCGH4 [II]] were synthesized from pentamethoxychalcone and 2,3,4,6-(OH) 4CGHCMe, resp. II was completely identical with the methylated derivative of aglycon of safflomin C, a constituent of safflower (Carthamus tinterorius L).

133466-24-7P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
133466-24-7 CAPLUS
Benzenepropanolic acid, 4-methoxy-a-[2,3,4,6-tetramethoxy-5-[3-(4-methoxyphenyl)-1-oxo-2-propenyl]phenyl]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 76 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1991:142803 CAPLUS
114:142803 CAPLUS
114:142803 CAPLUS
Synthesis of methyl 2,3-diaryl-3-methoxypropanoates by oxidative
rearrangement of chalcones using hypervalent iodine reagents in trimethyl
orthoformate
Singh, Om V.; Garg, Chandra P.; Kapoor, Ram P.
Dep. Chem., Kurukshetra Univ., Kurukshetra, 132 119, India
Synthesis (1990). (11), 1025-6
CODEN: SYNTBF: ISSN: 0039-7881
JOURNAL
JOURNAL
English
CASREACT 114:142803

A diastereoselective synthesis of Me 2,3-diaryl-3-methoxypropanoates I (R = Ph, 4-ClCGH4, Rl = Ph, 4-MeOCGH4, 4-MeCGH4) by oxidative rearrangement of RicoCH:CHR with (diacetoxyiodo)benzene and hydroxy(tosyloxy)iodobenzene in CH(OME) 3 is described.
132814-43-8F 132814-45-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
132814-43-8 CAPLUS
Benzenepropanoic acid, a-(4-chlorophenyl)-8,4-dimethoxy-,
methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

132814-45-0 CAPLUS Benzenepropanoic acid, α -(4-chlorophenyl)- β -methoxy-4-methyl-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 75 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 76 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 77 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1991:13787 CAPLUS
114:13787
Electrochemistry of some ethyl e-bromo(dihalophenyl) acetates and
electrochemical synthesis of diastereoisomeric diethyl
2,3-bis(dihalophenyl) succinates
Nattiello, Leonardo: De Luca, Carlo: Rampazzo, Liliana
Cent. Stud. Elettrochim. Chim. Fis. Interfasi, CNR, Rome, Italy
Journal of the Chemical Society, Perkin Transactions 2: Physical Organic
Chemistry (1972-1999) (1990), (6), 1041-4
CODEN: JCPKEH: ISSN: 0300-9580
JOURNal
English
Et e-bromo-2,4- or -3,4-dihalogenophenylacetates (ABr), where
halogen = F or Cl, are prepared and electrolyzed on reticulated vitreous C
(RVC) in DMF containing EtanClod (0.1 mol dm-3). Potentiostatic reduction

(RVC) in DMF containing EtANClO4 (0.1 mol dm-3). Potentiostatic reduction 5 --1.6 to -1.8 V vs. SCE furnishes the corresponding racemic and meso succinates. Monoesters are also isolated. An excess of racemic isomers is observed for some compds. Voltammetric expts. show practically no difference between the reduction potentials of the isomeric compds. Disastereoisomers can be distinguished by NNR spectroscopy, allowing disastereoisomeric excess to be evaluated before isolation of the single products. A mechanism involving radical intermediates cannot be excluded. On this basis, the disstereoisomeric excess can be explained by assuming different geometries for radical intermediates when the Ph group bears different substituents for radical intermediates when the Ph group bears 129430-58-6P 129430-59-7P 129430-60-0P 129430-61-1P 129430-62-2P 129430-63-3P 129430-64-4P 131003-67-1P RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in electrochem. reduction of bromodihalogenophenyl esters) 129430-58-6 CAPLUS Butanedioic acid, 2,3-bis(2,4-dichlorophenyl)-, diethyl ester, (R*,5*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

129430-59-7 CAPLUS Butanedioic acid, 2,3-bis(2,4-dichlorophenyl)-, diethyl ester, (R^*,R^*) -(9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 77 OF 146 CAPLUS COPYRIGHT 2007 ACS On STN (Continued)

129430-63-3 CAPLUS Butanedioic acid, 2,3-bis(3,4-dichlorophenyl)-, diethyl ester, (R*,R*)-(SCI) (CA INDEX NAME)

Relative stereochemistry.

129430-64-4 CAPLUS Butamedicic acid, 2,3-bis(3,4-difluorophenyl)-, diethyl ester, (R*,5*)-(9C1) (CA INDEX NAME)

Relative stereochemistry.

131009-67-1 CAPLUS
Butanedioic acid, 2,3-bis(3,4-difluorophenyl)-, diethyl ester, (R*,R*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 77 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

129430-60-0 CAPLUS Butanedioic acid, 2,3-bis(2,4-difluorophenyl)-, diethyl ester, (R*,S*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

129430-61-1 CAPLUS Butanedioic acid, 2,3-bis(2,4-difluorophenyl)-, diethyl ester, (R*,R*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

129430-62-2 CAPLUS Butanedioic acid, 2,3-bis(3,4-dichlorophenyl)-, diethyl ester, (R*,5*)-(9CI) (CA INDEX NAME).

Relative stereochemistry.

ANSWER 77 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 78 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1990:198049 CAPLUS 112:198049
Preparation of some chromans substituted at the 3- or 4-position by an aryl or benzyl group by the rhodium-catalyzed intramolecular nucleophilic substitution of the corresponding 3-(2-fluorophenyl)propan-1-ols Houghton, Roy P.: Shervington, Leroy A. Coll. Cardiff, Univ. Wales, Cardiff, CPI 3TB, UK Journal of Chemical Research, Synopses (1989), (8), 239 CODEN: JRPSDC: ISSN: 0308-2342 Journal English CASREACT 112:198049

[Rh(n5-C5ELMe4) (n6-C6H6)][PF6]2 catalyzed the formation of chromans (I, R = H, CH2OH, Ph, 2-FC6H4, CH2Ph; R1 = Ph, 4-02NC6H4, 4-MeCC6H4, CH2OH, H) from 2-FC6H4CHRCHR1CH2OH in MeN02-Me2CO. 126348-14-99 126348-14-9r
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent) SYN (Synthetic preparation), FREF (Freparation), (Reactant or reagent) (preparation and reduction of) 126348-14-9 CAPUS
Butanedioic acid, 2,3-bis(2-fluorophenyl)-, dimethyl ester (9CI) (CA

ANSWER 80 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1988:473717 CAPLUS 109:73717

109:73717
Stereoselective synthesis of the dihydrobenzo[b]furan segments of the ephedradine alkaloids
Baker, Raymond: Cooke, Nigel G.; Humphrey, Guy R.; Wright, Stanley H. B.; Hirshfield, Jordan
Dep. Chem., Univ. Southampton, Southampton, SO9 5NH, UK
Journal of the Chemical Society, Chemical Communications (1987), (14), 1102-4

CODEN: JCCCAT: ISSN: 0022-4936

Journal English CASREACT 109:73717

Dihydrobenzofuran derivs. I (R, R1 = H, MeO; R2 = H, Me) were prepared via Levis-catalyzed cyclization of phenol substituted β-hydroxy esters II as key step; the use of chiral loxazolidinones in the aldol reaction has formed the basis of enantiospecific syntheses of III (R3 = CO2Me, CH2OH). 115439-21-pp 115439-22-0p 115439-23-1p 115439-23-Pp 115439-25-3P 115439-27-Fp 115439-28-6P 115439-27-Fp 115439-28-6P 115439-27-Pp 115439-28-6P 115439-27-Fp

115465-67-3P
RE: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(Repreparation and intramol. cyclization of, benzofuran derivative from)
115439-21-9 CAPLUS
Benzenepropanoic acid, a-{5-{dimethoxymethyl}-2-{phenylaethoxyyphenyl}-β,4-dihydroxy-, methyl ester, (R*,R*)- (9CI)
(CA INDEX NAME)

Relative stereochemistry

ANSWER 79 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1990:178248 CAPLUS 112:178248 112:178248 CAPLUS 112:178248 Synthesis and some reactions of [Z]-methyl \(\alpha - [2-\text{o}-carboxyphenyl] - m-chlorocinnamate Mahmoud, M. R. Fac. Sci., Ain shams Univ., Cairo, Egypt Journal of the Chemical Society of Pakistan (1989), 11(2), 144-50 CODEN: JCSPDF: ISSN: 0253-5106 Journal English CASREACT 112:178248

AB (Z)-2-H02CCGH4C(C02R):CHCGH4Cl-3 (I: R = Me)(II) was heated with aqueous NaOH

to give the dibasic acid I (R = H), which was converted to the cyclic anhydrides (2)-III (IV) and (E)-III. IV was cyclized with AlCl3 to give indenyl acid V. Bromination, lactonization and cyclization of II was studied. The reaction of II and IV with primary amines, hydroxylamine, hydroxylamine, hydroxylamine, hydroxylamine were also investigated. 126558-65-4Physics and p-nitrophenylhydrazine were also investigated. RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 126558-65-4 CAPIUS
Benzenepropanoic acid, α,β-dibromo-α-(2-carboxyphenyl)-3-chloro-, monomethyl ester (9CI) (CA INDEX NAME)

ANSWER 80 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

115439-22-0 CAPLUS

Benzemeropanoic acid, e-[5-(dimethoxymethyl)-2-(phenylmethoxy) phenyl]-B, 4-dihydroxy-3-methoxy-, methyl ester, (R,S*)-(9C1) (CA INDEX NAME).

Relative stereochemistry.

115439-23-1 CAPLUS Benzenepropanoic acid, α -[5-(dimethoxymethyl)-2-(phenylmethoxy)phenyl)- β , 4-dihydroxy-3-methoxy-, methyl ester, $\{R^+,R^+\}$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

115439-24-2 CAPLUS
Benzenepropanoic acid. a-{5-(dimethoxymethyl)-2-

ANSWER 80 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (phenylmethoxy) phenyl]- β -hydroxy-3,4-dimethoxy-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

115439-25-3 CAPLUS

BenZenepropanoic acid, α -[5-(dimethoxymethyl)-2-(phenylmethoxy) phenyl]-8-hydroxy-3,4-dimethoxy-, methyl ester, (R,R)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

115439-26-4 CAPLUS Benzenepropanoic acid, α -{5-(dimethoxymethyl}-3-methoxy-2-(phenylmethoxy)phenyl}- β ,4-dihydroxy-, methyl ester, { R^* , S^* }- {9CI} (CA INDEX NAME)

Relative stereochemistry.

ANSWER 80 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (phenylmethoxy) phenyl]-B-hydroxy-4-methoxy-, methyl ester, (R*,R*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

115465-67-3 CAPLUS Benzenepropanoic acid, α -{5-(dimethoxymethyl)-2-(phenylmethoxy)phenyl]- β ,4-dihydroxy-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 80 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

115439-27-5 CAPLUS
Benzenepropancic acid, α -[5-(dimethoxymethyl)-3-methoxy-2(phenylmethoxy)phenyl]- β ,4-dihydroxy-, methyl ester, (R*,R*)- (9CI)
(CA INDEX NAME)

Relative stereochemistry.

115439-28-6 CAPLUS
Benzenepropanoic acid, a-[5-(dimethoxymethyl)-2-(phenylmethoxy)phenyl]-B-hydroxy-4-methoxy-, methyl ester, (R*,S*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

115439-29-7 CAPLUS Benzenepropanoic acid, α -[5-(dimethoxymethyl)-2-

L4 AN DN TI

AU CS SO

ANSWER 81 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1988:131218 CAPLUS
108:131218 CAPLUS
108:131218 CAPLUS
108:131218 CAPLUS
108:131218 CAPLUS
1108:131218 CAPLUS
1108:

electrolyzing di-Me bromomalonate and related tompass in absolutions containing
0.1M Ba(Cl04)2 as electrolyte on nickel cathode at controlled potential.
A suitable mechanism.involving the formation of malonate carbanion intermediate is suggested.

IT 34404-72-3 34404-73-4P
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of)
RN 34404-72-3 CAPLUS
CN 1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetramethylester (9CI) (CA INDEX NAME)

34404-73-4 CAPLUS
1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-chlorophenyl)-, tetramethyl ester (9C1) (CA INDEX NAME)

ANSWER 82 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1988:131203 CAPLUS
108:131203 cAPL

Electrochem. reduction of 4-RC6H4CHBrCO2Et (I, R = Br, Cl, F) gave the (i)-and meso-isomer of 4-RC6H4CH(CO2Et)CH(CO2Et)CH9R-4, epoxides II, and 4-RC6H4CH2CO2Et. The (i)- and meso-isomers were identified by MMR

4-RCDMCHCOZET. The (+)- and meso-isomers were identified by NMR spectroscopy.
113387-87-4P 113387-88-5P 113387-90-9P 113387-91-0P 113387-91-2P 113387-91-2P 113387-91-2P 113387-91-2P 113387-91-2P 113387-91-2P 113387-91-2P 113387-81-4CAPLUS

Butanedioic acid, 2,3-bis(4-fluorophenyl)-, diethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

113387-88-5 CAPLUS

Butanedioic acid, 2,3-bis(4-fluorophenyl)-, diethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 82 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

113387-94-3 CAPLUS Butanedioic acid, 2,3-bis(4-bromophenyl)-, diethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry

ANSWER 82 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

113387-90-9 CAPLUS

Butanedioic acid, 2,3-bis(4-chlorophenyl)-, diethyl ester, (R*,5*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

113387-91-0 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-, diethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

113387-93-2 CAPLUS Butanedioic acid, 2,3-bis(4-bromophenyl)-, diethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 83 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1987:635925 CAPLUS
107:235925
The different recombinations of diphenylmethyl radicals, Ph2C(-)R
(R = CMe3 CN, COZR', COR')
Neumann, W. P.; Stapel, R.
Univ. Dortmund, Dortmund, D-4600/50, Fed. Rep. Ger.
NATO ASI Series, Series C: Mathematical and Physical Sciences (1986),
189 (Substituent Eff. Radical hohem), 219-22
CODEN: NSCSDW; ISSN: 0258-2023
Journal
English
ESR data for radicals RZICR+ (R1 = Ph, p-anisyl, p-tert-butylphenyl; R
- Me3C, SiMe3, COZMe, COZET, COZCHZPh, CHO, COPh, etc.) and dissociation
enthalpies of their dimers are measured.
104505-55-7
LRPUR (Properties)
(dissociation enthalpy of)
104505-55-7 CAPLUS
Butanedioic acid, tetrakis[4-(1,1-dimethylethyl)phenyl]-, dimethyl ester
(9CI) (CA INDEX NAME)

ANSWER 84 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1987:196146 CAPLUS
106:196146
Estrogenic affinity labels: synthesis, irreversible receptor binding, and bioactivity of aziridine-substituted hexestrol derivatives
Zablocki, Jeffery A.; Katzenellenbogen, Jenna S.;
Norman, H. J.; Katzenellenbogen, Benita S.
Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA
Journal of Medicinal Chemistry (1987), 30(5), 829-38
CODEN: JMCAR: ISSN: 0022-2623
JOURNAL
English
CASREACT 106:196146

Aziridine derivs. (e.g., I) of the potent nonsteroidal estrogen hexestrol [(3R*,45*)-3,4-bis(4-hydroxyphenyl)hexane] were prepared as affinity labels for the estrogen receptor that are estrogen agonists, rather than antagonists. Thus, the mesylate II was treated with ethylenimine to give 50% 1. In these compds. the hexestrol ligand and the aziridine are linked by a carbonyl group (ketone or estet), a thio ether, or a methylene chain. The apparent competitive binding affinity of these derivs. for the estrogen receptor ranges from 1.8% to 25% that of estradiol, and most of them bind in a time-dependent, irreversible manner with the receptor, although the rate and efficiency of this binding vary widely, often with relatively small changes in structure. This is consistent with the irreversible attachment requiring a precise alignment of activating and reacting residues in the binding site of the receptor. The estrogenic and antiestrogenic activity of these aziridine derivs. was investigated in MCF-7 human breast cancer cells. Most of the compds. are agonists, with one being an antagonist. I has the most ideal behavior of the estrogenic affinity labeling agents prepared It is an agonist, and it binds to receptor irreversibly, efficiently, and quite rapidly. 107036-27-1P 107036-28-2P RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Beactant): S

Relative stereochemistry.

ANSWER 84 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Contine Benzenepropanoic acid, \$\textit{\beta}\-ethyl-4-hydroxy-a-(4-hydroxyphenyl)-,}{2-(1-aziridinyl)ethyl ester, \$(R^*,S^*)-(9CI)} (CA INDEX NAME) (Continued)

Relative stereochemistry.

ANSWER 84 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

107036-28-2 CAPLUS
Benzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-,
2-iodoethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

107036-09-9P 107036-10-2P

RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation and estrogen receptor binding affinity and agonist activity

107036-09-9 CAPLUS

Benzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-, 3-(1-aziridinyl)propyl ester, (R*,5*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

107036-10-2 CAPLUS

ANSWER 85 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1987:66855 CAPLUS 106:66855

106:66855
Sterically hindered free radicals. XVI. The existence of tetraphenylsuccinic acid and its esters, and the structur of the diarylmethyl radicals R2C=X (X = CO2R1, CN, COR1) Neumann, Wilhelm P., Stapel, Ralf Univ. Dortmund, Dortmund, D-4600/50, Fed. Rep. Ger. Chemische Berichte (1986), 119(11), 3422-31 CODEN: CHBEAM; ISSN: 0009-2940 JOHNBAL CASTALL ture of the dimers

CS SO

CASREACT 106: 66855

The coupling of Ph2CBrCO2Et in refluxing C6H6 containing Cu powder followed

rearrangement and deesterification gave 1,4-[Ph2C(CO2H)]CGH4. Also prepared were NeO2C(CGH4CNe3-4)2C(CGH4CNe3-4)2CO2Ne, Ph2CcCROCPh2COR (R = H, Ne, Ph), and di-Me 9,9'-bifluorene-9,9'-dicarboxylate. The ESR of R22C-R3 (R2 = Ph, 4-Me3CCGH4; R3 = CO2Ne, cyano, CHO, Ac, B2) and heats of dissociation of the radical dimers were determined 104505-55-7p

IT

ANSWER 86 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1986:206811 CAPLUS 104:206811 104:206811
Reactions with stable phenoxyl radicals De Jonge, Cornelis R. H. I. Corp. Res. Dep., Akzo Res., Arnhem, Neth. Liebigs Annalen der Chemie (1986), (2), 299-304 CODEN: LACHDL; ISSN: 0170-2041 Journal Control of C

Phenoxyl radical I was generated and underwent H abstraction reactions with Me, methylene, and methine compds, to form ethers. Triply activated compds. PACHCN and p-MecGH4CH(CN)COZMe underwent C-C dimerization on treatment with I. 31249-03-3P

ĪТ

31249-03-3P
RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
31249-03-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester
(9CI) (CA INDEX NAME)

ANSWER 87 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 87 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1986:148061 CAPLUS
104:148061 CAPLUS
104:148061 CAPLUS
104:148061 CAPLUS
104:148061 CAPLUS
104:148061 CAPLUS
105:148061 CAPLUS
105:148061 CAPLUS
106:148061 CAPLUS
106:148061 CAPLUS
106:148061 CAPLUS
106:148061 CAPLUS
106:148061 CAPLUS
107:148061 CAPL AU CS SO English CASREACT 104:148061

The anodic coupling reactions of 4-benzylisochromanone I and 4-benzyl-1,2,3,4-tetrahydroisoquinolines II (R = Me, RI = H: R= Me, CO2Et, CHO, RI = OMe) were studied and compared. In neutral media II gave products of coupling to C-1 and/or N-2, depending on the ring substituents. In acid solution, II gave isoaporphines, whereas the 1-benzyl analogs couple at C-8 ato give morphinedienones. The different regionelectivities are due to inductive effects in the protonated bases. I also couples at C-8 but the resulting, intermediate is unstable and reacts further with nucleophiles to give 24% 2,5-(OHC) (MeO/CHGCHGHOWHO-13 and 6.3% phenanthrene III. 98748-60-8P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, by regionelective anodic oxidation-ring cleavage of isochromanones) 98748-60-8 CARLUS
Benzenepropanoic acid, α-(2-formyl-5-methoxyphenyl)-3-methoxy-, Benzenepropanoic acid, α -(2-formyl-5-methoxyphenyl)-3-methoxy-, methyl ester (CA INDEX NAME)

ANSWER 88 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1995:45575 CAPLUS
102:45575
102:1573a,7160a
Synthetic studies in polycyclic systems: part IX - synthesis of methoxy derivatives of 11H-benzo[a]fluorenes and 11H-naphtho[2,1-a]fluorenes
Rao, Alaka: Lala, Sunandan: Rao, R. R.
Dep. Chem., Yisva-Bharati Univ., Santinietan, 731 235, India
Indian Journal of Chemistry, Section B: Organic Chemistry Including
Medicinal Chemistry (1984), 238(7), 603-10
CODEN: 1585DB; ISSN: 0376-4699
Journal
English
CASREACT 102:45575

Michael reaction of RCH:CHCO2Et (R = CGH4CMe-2, -3, -3,CGH3COMe)2-3,4] with R1CH2CO2Et (R1 = Ph, 2-naphthyl) gave 75-868 EtO2CCHR1CHRCH2CO2Et, which was hydrolyzed to give HO2CCHR1CNRCH2CO2Et. The diacids were cyclized with SnCl4 to give 54-648 tetrallend edrivs. 1 (R2 = R3 = H, CH:CHCH:CH: X = 0) which were reduced with Zn or HZNNHZ to give 58-67, 59-668 I (X = H2) resp. The last were methylated, dehydrogenated, and saponified to give naphthalene- and phenanthrenecarboxylic acids II (same R's), which were cyclized using HZSO4, AlCl3, or SnCl4 to give 18-38, 29-42, 52-744 fluorenone derivs. III (R4 = R6 = OMe, R3 = H; R4 = OMe, R5 = R6 = H; R5 = CMe; R4 = R5 = H, R6 = OMe, R5 = R6 = H; R5 = CMe; R4 = R5 = H, R6 = OMe, R5 = R7 = X = H2), 94146-62-0P
RL: RCT (Reactant); SFN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and saponification of) 94146-62-0 CAPLUS
Pentamedioic acid, 2-(2-(ethoxycarbonyl)phenyl]-3-(2-methoxyphenyl)-, diethyl ester (9CI) (CA INDEX NAME)

ANSWER 88 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 94146-63-1P 94146-64-2P 94146-65-3P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation, hydrolysis, and Dieckmann cyclization of)
RN 94146-63-1 CAPLUS
CN Pentamedioic acid, 2-[2-(ethoxycarbonyl)phenyl]-3-(3-methoxyphenyl)-, diethyl ester (9CI) (CA INDEX NAME)

94146-64-2 CAPLUS Pentamedioic acid, 2-[2-(ethoxycarbonyl)phenyl]-3-(4-methoxyphenyl)-, diethyl ester (9C1) (CA INDEX NAME)

94146-65-3 CAPLUS ysiso-bb-3 CAPLUS Pentanedioic acid, 3-(3,4-dimethoxyphenyl)-2-[2-(ethoxycarbonyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 89 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1984:120280 CAPLUS
DN 100:120280
CORET 100:120280
TELECTROCHEMICAL SYNTHOSIS OF 5,6,11,12-tetrahydro-5,6,11,12-tetrakis (ethoxycarbonyl)dibenzo[s,e]cyclooctene
AU De Luca, Carlor Inesi, Achiller Rampasso, Liliana
C Cent. Stud. Elettrochim. Chim. Fis. Interfasi, CNR Roma, Rome, Italy
Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1981), (12), 1821-5
CDDEN: JCPKBH: ISSN: 0300-9580
DJ Journal
LA English
GI

DT LA GI

CO2Et CO2Et

CO2Et

Electrochem. reduction of 1,2-{Et02CCHBr}}2C6H4 {I) in DMF at a vitreous C electrode gave 15% 1,2-{Et02CCH2}}2C6H4, 16% title compound (II), 16% [o-Et02CCH2C6H4CH(COZET)]2 and 20% polymer as the major products. Only apprx.N1 of benzocyclobutene III was formed. The intermediate formation of c,a'-bis(ethoxycarbonyl)-o-quinodimethane, whose behavior resembles that of a biradical, through the 2 electron electrochem. reductive elimination of the Br- ions from I, is the key step in this reaction.

89215-22-5P 89215-23-6P 89215-24-7P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

89215-22-5 CAPLUS
Butanedioic acid, 2,3-bis[2-{2-ethoxy-2-oxoethyl}phenyl}-, diethyl ester, (R*,5%)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 88 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

L4 ANSWER 89 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN Relative stereochemistry. (Continued)

89215-24-7 CAPLUS 1,2-Benzenedipropanoic acid, β,β' -bis(ethoxycarbonyl)- α,α' -bis[-2(-2-ethoxy-2-oxoethyl)phenyl]-, diethyl ester, $(\alpha R^*,\alpha'R^*,\beta R^*,\beta'R^*)$ - (9CI) (CA INDEX NAME)

ANSWER 90 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1983:453253 CAPLUS
DN 99:53253
OREF 99:8309a
TI The sensitized photooxidation of methyl (E)-ferulate
AU Kuo, Yueh Hsiung: Kuo, Pao Chu: Lin, Sheng Tsair
CS Dep. Chem., Natl. Taiwan Univ., Taipei, Taiwan
Froceedings of the National Science Council, Republic of China, Part B:
Basic Science (1981), 7(1), 28-34
CODEN: PCRCO3; ISSN: 0253-6070
D Journal

Journal English

The title reaction gave 4 products, Me (2)-ferulate, vanillin, I, and II. Product structures were elucidated by chemical derivs. 86069-39-86069-40-1P

ΙT

86069-39-8P 86069-40-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
86069-39-8 CAPLUS
Benzenepropanoic acid, 4-hydroxy-a-{2-hydroxy-3-methoxy-5-{3-methoxy-3-oxopropyl)phenyl}-3-methoxy-, methyl ester (CA INDEX NAME)

86069-40-1 CAPLUS

Benzenepropanoic acid, 4-{acetyloxy}-a-[2-(acetyloxy)-3-methoxy-5-(3-methoxy-3-oxopropyl)phenyl]-3-methoxy-, methyl ester (CA INDEX NAME)

ANSWER 91 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1983:218134 OAPLUS
98:218134 98:31155a,33156a
Fluorescent chelates and labeled specific binding reagents prepared from
them
Hinshaw, Jerald Clyder Toner, John Luke: Reynolds, George Arthur
Eastman Kodak Co., USA
EUr. Pat. Appl., 50 pp.
COLEN: EPXXDW
Patent
English
CMT 2

170	Engitan				
FAN.	CNT 2				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 68875	A2	19830105	EP 1982-303380	19820628
	EP 68875	A3	19830504		
	EP 68975	Bl	19871223		
	R: DE, FR, GB				
	CA 1205028	A1	19860527	CA 1982-405050	19820611
	JP 58009783	A	19830118	JP 1982-112653	19820701
	JP 06014042	В	19940223		
	US 4637988	λ	19870120	US 1986-825693	19860203
	US 4670572	A	19870602	US 1986-825009	19860203
	US 4801722	λ	19890131	US 1987-7024	19870127
	US 4794191	A	19881227	US 1988-151847	19880203
	US 4859777	Α	19890822	US 1988-285163	19881216
PRAI	US 1981-279398	A	19810701		
	US 1986-825693	A3	19860203		
	US 1987-7024	A3	19870127		
	US 1987-40385	A3	19870420		

Uniperiodes As 1987-409
CASREACT 98:218134; MARPAT 98:218134
Stable fluorescent chelates are manufactured comprising a complex of a lanthandde metal and a chelating agent that includes a monety that is a triplet sensitizer having a triplet energy greater than that of the lanthandde metal and at least 2 heteroatom-containing groups that form coordinate complexes with lanthanide metals and a 3rd heteroatom-containing group or heteroatom in or appended to the triplet sensitizer. Thus, a benzoylhydroxybis(N.Ph.bis(Carboxylate)aminomethyl)coumarin-Eu chelate was used with an anal. test element containing oxibimin and normal rabbit serum and the fluorescence signal was a function of the concentration of the Euchelate. The chelate is useful to label a variety of physiol. active materials by binding them to the complex by adsorption or by covalent bonding. The materials are especially useful in specific binding assay codes.

bonding. The materials are especially useful in specific binding assay methods.

IT 85929-38-0P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 85929-38-0 CAPUSO,
CN Benzenepropanoic acid, a-[3-[4-(acetyloxy)-3,5-bis[[bis[2-(1,1-dimethylehoxy)-2-oxocthyl]maino]methyl]benzoyl]phenyl]-4-(4-hydroxy-3,5-diiodophenoxy)-3,5-diiodo-, methyl ester (CA INDEX NAME)

ANSWER 90 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 91 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN PAGE 1-A

PAGE 1-B

85916-19-4P
RL: PREP (Preparation)
(preparation of)
85916-19-4 CAPLUS
Benzenepropanoic acid, α -[3-[3,5-bis[[bis(carboxymethyl)amino]methyl]
1-4-hydroxybenzoyl]phenyl]-4-(4-hydroxy-3,5-diiodophenoxy)-3,5-diiodo-, α -methyl ester (9CI) (CA INDEX NAME)

ANSWER 92 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1981:88667 CAPLUS
98:88867
98:13847a.13550a
Thermal, photochemical, and acid-catalyzed rearrangements of the spiro
dimer of a,a'-bis(methoxycarbonyl)-o-quinodimethane. X-ray
crystal structure of trans,trans-retrakis(methoxycarbonyl)dibenzo[a,e]cycl
ooctene
Jones, David W., McDonald, Walter S.
Dep. Org. Chem., Univ. Leeds, Leeds, Ls2 9JT, UK
Journal of the Chemical Society, Perkin Transactions 1: Organic and
Bio-Organic Chemistry (1972-1999) (1982), (9), 2257-63
CODEN: JCPRB4; ISSN: 0300-922X
Journal
English

The stereochem. of the title spiro-dimer I (R = R2 = CO2Me, R1 = R3 = $\{II\}$ was determined by comparison of its properties with those of the

As the state of th

ANSWER 92 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) 84198-36-7 CAPLUS (Continued)

1,2-Benzenediacetic acid, α -[2-methoxy-1-[2-(2-methoxy-2-oxoethyl]- α '-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)

84198-40-3 CAPLUS 1,2-Benzenediacetic acid, $\alpha-[2-methoxy-1-[2-(2-methoxy-2-oxoethyl)phenyl]-2-oxoethyl]-, dimethyl ester, <math>(R^*,R^*)-$ (9CI) (CA INDEX

Relative stereochemistry.

ANSWER 92 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continue 1,2-Benzenediacetic acid, α -[2-methoxy-1-[2-(2-methoxy-2-cxoethyl)phenyl]-2-cxoethyl]- α -"[[(4-methytphenyl)sulfonyl]oxy]-, dimethyl ester, [α R*(R*), α *S*]- (9C1) (CA INDEX NAME) (Continued)

84275-76-3 CAPLUS
1,2-Benzenediacetic acid, a-[2-methoxy-1-[2-(2-methoxy-2-oxoethyl]-a'-[[(4-methylphenyl)=ulfonyl]oxy]-,
dimethyl ester, [aR'(R'),a'R']- (9CI) (CA INDEX NAME)

84198-36-7P 84198-40-3F

ANSWER 93 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1982:556714 CAPLUS 97:156714 97:156714 97:156714 97:25985a, 25988a (2R*,35*)-1-[1251]Iodo-2,3-bis(4-hydroxyphenyl)pentane ([1251]iodonorhexestrol), and (2R*,35*)-1-[77Br]bromo-2,3-bis(4-hydroxyphenyl)pentane ([77Br]bromonchexestrol), two \(\gamma\)-emitting estrogens that show receptor-mediated uptake by target tissues in vivo Landvatter, Scott W.: Katzenellenbogen, John A.: McElvany, Xaren D.: Welch, Mtchael J.
Sch. Chem. Sci., Univ. Illinois, Urbana, IL, 61801, USA Journal of Medicinal Chemistry (1982), 25(11), 1307-12 CODEN: JMCMAR: ISSN: 0022-2623 Journal English ΑU

CS SO

Two y-emitting estrogen analogs, (2R,3S)-1-[1251]iodo-2,3-bis(4-hydroxyphenyl)pentane (I) [83181-42-4] and (2R,3S)-1-[77Br]bromo-2,3-bis(4-dydroxyphenyl)pentane (II) [83181-42-5] were prepared by halide ion displacement on a labile trifluoromethanesulfonate derivative of a suitably protected precursor, followed by mild acid deprotection. Although halide displacement on a more stable tristrifluoromethanesulfonate derivative was successful, the basic conditions required for deprotection of this precursor resulted in destruction of the products by a base-induced spicoslimination reaction. In immature female rats, both of these halonorhexestrols demonstrated preferential uptake by the uterus that could be selectively blocked by coadministration of a large dose of unlabeled estradiol. In a double label comparison with [6e-[1251]iodo-176-estradiol, the uterine uptake of II was notably less selective. Stability studies in vitro and in vivo indicated that both I and II are quite labile, and this lability compromises the selectivity of their uptake by estrogen target tissues in vivo. p-Hydroxyphenethyl halides are known to be unusually prone to a base-catalyzed solvolysis, via cyclization of the phenolate to a spirocyclohexadienone intermediate. This unusual solvolytic mechanism may contribute to the lability of these halonorhexestrols in vivo. 83213-76-7 CAPLUS
BERIEROFFO (PARCET (Reactant): (CA INDEX NAME)
BERIEROFFO (PARCET) (CA INDEX NAME)

Benzenepropanoic acid, B-ethyl-4-hydroxy-q-(4-hydroxyphenyl)-, methyl ester, (R*,5*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 93 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 95 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1981:61:5317 CAPLUS 95:215317 95:35821a,35824a OREF TI Stereochemical considerations in the binding of nonsteroidal estrogens to Stereochemical considerations in the binding of nonsterd the estrogen receptor Landwatter, Scott W.; Katzenellenbogen, John A. Sch. Chem. Sci., Univ. Illinois, Urbana, IL, 61801, USA Molecular Pharmacology (1981), 20(1), 43-51 CODEN: MOPMA3; ISSN: 0026-895X Journal English

Derivs. of nonsteroidal estrogens, such as hexestrol, can interact with the estrogen receptor in 4 possible binding modes, 2 per enantiomer. Several side chain-functionalized hexestrol and norhexestrol derivs, have been synthesized and resolved into pure enantiomers. Binding studies with lamb uterine estrogen receptor have indicated that there is no appreciable difference in binding between enantiomers in the hexestrol series. Enantiomers in the norhexestrol series, on the other hand, do show differences in binding. The (-) (2R, 35)-pentyl ester (1) [79568-12-0] binds to receptor with twice the affinity of racemic material and 14 times the affinity of the (+) (2S, 3R)-antipode [79923-77-0]. It is concluded that the norhexestrols prefer 1 of the 4 possible binding modes, whereas the hexestrols can adopt 2 of the 4 modes equally. Furthermore, comparisons between the binding affinities of corresponding hexestrol and norhexestrol derivs. suggest that the source of chiral recognition is a specific interaction between the carbomyl group in the 2R,3S enantiomer of the norhexestrol derivs. that elevates affinity, this interaction not being attainable in the other enantiomer and in the derivs. in the hexestrol series.

79568-12-07 79618-13-06 79618-14-7P
79645-19-59 83213-76-7P
RL: SPN (Synthetic preparation); PREF (Preparation) (preparation and estrogen receptor binding of)
79568-12-O CAPLUS
Benzenepropanoic acid, β-ethyl-4-hydroxy-a-(4-hydroxyphenyl)-, nearly leafs. (R-6.8-S)1-(9.71) (CA INDEX NAME)

Benzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-, pentyl ester, [R-(R*,S*)]- (9Cl) (CA INDEX NAME)

Absolute stereochemistry.

ANSVER 94 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1982:527210 CAPLUS
DN 97:127210
OREF 97:21105a, 21108a

II Uncatalyzed insertion reaction of isocyanides into a carbon-sulfur bond
AN Morel, G.: Marchand, E.: Mguyen Thi, K. H.: Foucaud, A.

CS Groupe Physiochim. Struct., Univ. Rennes, Rennes, 35042, Fr.

Tetrahedron Letters (1982), 23(19), 2023-6

COODE: TELEAY: ISSN: 0040-4039

UT Journal
L English
OS CASREACT 97:127210
AB RNC (I: R = Me3C, tert-octyl) with RIC(CN) (SR2)CO2Me (II: R1 = Ph2C(CN), R2 = Me, Ph, PhCH2: R1 = 5-cyanofluoren-5-yl. (PhCH2)2C(CN), PhCMe(CN), PhCEC(CN), R2 = Me] at room temperature for 17-114 h gave 36-844

RN:C(SR2)CR1(CN)CO2Me (III). III (R2 = Ph) are unstable and rearrange at room temperature to give E- and Z-RN(CO2Me)C(SR2):CR1(CN) (E-Z-IV) in 6-82% yield. I with II [R] = p-R3C6H4 (R3 = C1, Me, MeO, NO2), PhCH2, R2 = Me; R1 = p-MeC6H4, R2 = PhCH2; R1 = R2 = Ph] in reluxing MeCN gave the corresponding E- and Z-IV in 19-94% yield.
31249-03-3. PRL: SFN (Synthetic preparation); PREP (Preparation) (preparation of) 31249-03-3 CAPLUS Butanediotic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)

ANSWER 95 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

79618-13-6 CAPLUS

Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, methyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

79618-14-7 CAPLUS Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, methyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

79645-19-5 CAPLUS Benzenepropanoic acid, β-ethyl-4-hydroxy-α-(4-hydroxyphenyl)-, pentyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 83213-76-7 CAPLUS

ANSWER 95 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Benzenepropanoic acid, β -ethyl-4-hydroxy- α -(4-hydroxyphenyl)-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

AN	1981:30582 CAPLUS	5			
DN	94:30582				
OREF	94:5043a,5046a				
TI	Homophthalimides	parrying	amino subst	ituents in the 2-positi	on
IN	Kutter, Eberhard;	Austel,	Volkhard: E	berlein, Wolfgang: Heid	er, Joachim
	Kobinger, Walter:	Lillie,	Christian;	Kadatz, Rudolf	
PA	Thomae, Dr. Karl,	G.m.b.H	., Fed. Rep.	Ger.	
so	Can., 74 pp.				
	CODEN: CAXXA4				
DT	Patent				
LA	English				
FAN.	CNT 3				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 1076116	A1	19800422	CA 1976-258095	19760729
	DE 2533986	A1	19770217	DE 1975-2533986	19750730
	DE 2533986	B2	19790906		
	DE 2533986	C3	19800522		
	DE 2622690	A1	19771208	DE 1976-2622690	19760521
PRAI	DE 1975-2533986	A	19750730		
	DE 1976-2622690	A	19760521		

L4 ANSWER 97 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

Amines I (X, XI = C2-4 alkylene, optionally substituted by Me or Ph; R, Rl, R7, R8 = H, F, Cl, Br, OH, NH2, NH2, NH2c, alkyl, alkony, alkylthio; R2, R3, R5, R6 = H, alkyl, phenylalkyl, methoxyphenylalkyl; R2A3, R5X6 = alkylene; R4 = H, alkyl, phenylalkyl) were prepared Thus, 4,4-dimethyl-1,3-isochromandione was treated with MeN[(CH2)3NH2]2 to give 65% II. II had an antiarrhythmic EDSO 5.5 pg/mL measured on the refractory period of isolated guinea pig left auricle. 76065-15-1 RL: RCT (Reactant): RACT (Reactant or reagent) (saponification of) 76065-15-1 CAPIUS Benzenepropanoic acid, 4-methoxy-q-[2-(methoxycarbonyl)phenyl]-e-methyl-, methyl ester (CA INDEX NAME)

AU CS SO

ANSWER 96 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1981:569267 CAPLUS
95:169267
95:28301a,28304a
Studies of organosilicon compounds. XXIX. Reaction of hydroxyaldehydes and hydroxyketones with trialkylsilanes
Lapkin, I. 1.; Dvinskikh, V. V.
Perm. Gos. Univ., Perm. USSR
Zhurnal Obshchei Khimii (1981), 51(6), 1354-60
CODEN: ZOKHA4: ISSN: 0044-460X
Journal
Russian
CASREACT 95:169267
Fifteen benzyloxysilanes were prepared in 27-79% yields by the title reaction in the presence of Ni. Thus, heating p-HOCGH4CHO with Et35iH in C6H6 at 85-90° 2.5-3 h in the presence of colloidal Ni gave 59%
PHOCGH4CH2OSiEt3.
79523-76-55
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
19523-76-5 CAPLUS
BUTANESION (A Note of the property of the colloid of the preparation of)
19523-76-5 CAPLUS
BUTANESION (A Note of the preparation) (CA Note of the preparation) (CA Note of the preparation of)
19523-76-5 CAPLUS
BUTANESION (CA NOTE NAME)

IT

ANSWER 97 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSVER 98 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

N 1981:30534 CAPLUS

N 94:30534

TI Electrochemical oxidation of aromatic ethers. Part 6. Oxidation of 4-(3,4-dimethoxybenzyl)-6,7-dimethoxy-2-methyl-1,2,3,4-tetrahydroisoquinoline and attempted synthesis of 4-(3,4-dimethoxybenzyl)-6,7-dimethoxy-2-methyl-1,4-dihydro-3(2H)-isoquinoline)

AU Carmody, Haurice P., Sainsbury, Halcolm, Newton, Roger F.

Sch. Chem., Univ. Bath, Bath, BAZ TAY, UK

SU Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1980), (9), 2013-20

CODEN: JCPRB4; ISSN: 0300-922X

JUNIAL English

English

Anodic oxidation at 1.15 and 1.9 V, resp., of the title tetrahydroisoquinoline (Bu4NBF4, CF3COZH-CH2CI2, C-felt anode, .apprx.3 h) gave the dihydroisoquinolinium derivs. I (R = H, RZ = bond, resp.), and no aryl-aryl coupled products were isolated. It is suggested that to achieve intramol. coupling of the 2 methoxylated rings their oxidation potentials should be closely similar. Cyclization of the amide II (Etpolyphosphoric ester, 140°, 15 min) gave the dibenzocycloheptene III (71%), and not the expected title dihydroisoquinolone. 76056-00-3P
RL: RCT (Reactant): SFN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)

- ANSWER 99 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1980:532199 CAPLUS 93:132199 93:21069a,21072a

- AU

- 93:132199
 93:21069a,21072a
 Thallium in organic synthesis. 57. Reaction of chalcones and chalcone ketals with thallium(III) trinitrate Taylor, Echvard C.; Conley, Richard A.; Johnson, David K.; McKillop, Alexander; Ford, Michael E.

 Dep. Chem., Princeton Univ., Princeton, NJ, 08540, USA
 Journal of Organic Chemistry (1980), 45(17), 3433-6
 CODEN: JOCEAN; ISSN: 0022-3263
 Journal English
 CASREACT 93:132199
 Treatment of chalcones ArCH:CHCOAr' with Tl(NO3)3 in acidic MeOH or in HC(OMe)3 gave (MeO) 2CHCHArCOAr' (lowythallation-rearrangement) and/or MeOCHArCHAr'CO2Me (ketalization-onythallation-rearrangement) The effect of substituents on Ar and Ar' on the ratio of the above rearrangement 74007-60-67
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 74007-60-6 CAPLUS
 Benzenepropanoic acid, β-methoxy-4-methyl-α-(4-methylphenyl)-,
 methyl ester (CA INDEX NAME)

- L4
- RN CN
- ANSWER 98 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (prepn. and cyclization of) 76056-00-3 CAPLUS Benzenepropanoic acid, α -[2-(bromomethyl)-4,5-dimethoxyphenyl]-3,4-dimethoxy-, ethyl ester (CA INDEX NAME)

- L4 AN DN OREF TI
- ANSWER 100 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1980:516183 CAPLUS 93:116183 93:116183 93:18609a,18612a Synthesis of trimeric lignin model compound composed of β-0-4 and β-1 structures Namba, Hiroakir Nakatsubo, Fumiakir Higuchi, Takayoshi Wood Res. Inst., Kyoto Inst., Uji, 611, Japan Mokuzai Gakkaishi (1980), 26(6), 426-31 CODEN: MKZGA7: ISSN: 0021-4795 Journal English
- AU CS SO

- Trilignol (I) [13459-21-7], a major structure in lignin, was synthesized in 460 overall yield via reaction of Me 4-benzyloxy-5-methoxybenzeneacetate [16209-54-4] with erythro-4-[[4-(4-benzyloxy-3-methoxybenzeneacetate [16209-54-4] with erythro-4-[[4-(4-benzyloxy-3-methoxybenzenealdehyde [74613-61-9] (5 steps), and its structure was elucidated by chemical anal. and UV. IR, NMR, and mass spectroscopy. 74613-58-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 [preparation and acetylation of)
 74613-58-4 CAPIUS
 Benzenepropanolic acid, \$-hydroxy-4-[2-hydroxy-2-(4-hydroxy-3-methoxybenyl)-1-(hydroxymethyl)ethoxy)-a-(4-hydroxy-3-methoxybenyl)-3-methoxy-, methyl ester (CA INDEX NAME)

ANSWER 100 OF 146 CAPLUS COPYRIGHT 2007 ACS On STN

ANSWER 102 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1980:514097 CAPLUS 93:114097 DN 93:114097

OREF 93:18249a,18252a

TI New 2-phenyl-3-aminopropanic acid derivatives

AU Fisnerova, L.: Grimova, J.: Nemecek, O.

SVyzk. Ustav Farm. Blochem., Prague, 13060/3, Czech.

Cooko-Slovenska Farmacie (1979), 28(8), 326-30

COOK: CKFRAY; ISSN: 0009-0530

DJ Journal

LA Czech

CASREACT 93:114097 CASREACT 93:114097

4-RCGH4CH2CO2Et [R = H, Me, Cl, Me2CH, Me2CHCH2) added to 22 R1CH:NCGH4R2
[I: Rl = 4-Me2CHCGH4, 3,4-methylenedioxyphenyl, 2- and 4-ClCGH4, Ph,
4-FCGH4, 2-furyl: R2 = 4-Me, H, 3-Cl, 4-Cl, 3,4-methylenedioxy, 4-CO2Et)
in anhydrous Me2SO containing EtONa at room temperature to give 26
esponding
4-RCGH4(CO2Et)CHRINHCGH4R2 (II) in 28-81% yield. Theor., 4-RCGH4CH2CO2H
(R = H, O2N, Cl) added to 9 R1CH:NR3 (Rl = Ph, 3,4-methylenedioxyphenyl,
4-Me2CHCGH4, 4-CLCGH4: R3 = Me, CMH62, Bu) at 100° under N to give
9 corresponding 4-RCGH4CH(CO2H)CHRINHR3 (III) in 11-50% yield. I (Rl =
4-ClCGH4, 4-Me2CHCGH4, R2 = 3,4-methylenedioxy; Rl = 4-Me2CHCGH4, R2 =
4-CLCGH4, 4-Me2CHCGH4, R2 = 3,4-methylenedioxy; Rl = 4-Me2CHCGH4, R2 =
4-ClCGH4, 4-Me2CHCGH4, R2 = 3,4-methylenedioxy; Rl = 4-Me2CHCGH4, R2 =
4-ClC) were prepared by standard methods. The LD50 of II and III were >1 body weight II (R = H, Cl, Rl = 3,4-methylenedioxyphenyl, R2 = H, 4-Me, 4-Cl; R = R2 = H, Rl = 4-Me2CHCGH4) and III (R = H, Rl = 3,4-methylenedioxyphenyl, R3 = CIMe2, Bu; R = Cl, Rl = 4-Me2CHCGH4, R3 = Me) had weak antiinflammatory activity.

74760-33-1P
RL: SPN (Synthetic preparation); PREP (Préparation)
(preparation, toxicity and antiinflammatory activity of)

74760-33-1 CAPUS
Benzenepropanoic acid, 4-(1-methylethyl)-α-(4-methylphenyl)-β-(phenylamino)-, ethyl ester (CA INDEX NAME)

L4 ANSWER 101 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1980:516113 CAPLUS DN 93:116113 CAPLUS DN 93:1161 APPLICATION NO. DATE JP 55052335 19800416 JP 1978-125721 19781014 PI JP 61047868 PRAI JP 1978-125721 GI PVC [9002-86-2] plastisols containing I (R = CN, COZRI; RI = Cl-3 alkyl) as radical initiators gave baked coatings free from bubbles. For example, a PVC plastisol containing trimethylolpropane trimethacrylate [3290-92-4] (reactive plasticizer) 60, DOP 100, epoxidized soybean oil 3, CaCO3 200, a Sn stabilizer 2, and I (R = CN, RI = Me) (II) [31249-03-3] 12 phr was baked on tinplate at 120° to give a coating with better adhesion and lower bubble content than that using 1,1-bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane in place of II. J1249-03-3
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for crosslinking of PVC plastisol coatings)
31249-03-3 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester
(9C1) (CA INDEX NAME)

DT LA GI

Phenylcoumarans I (R, Rl = H, MeO) were prepared by introducing a 2C side chain to a vanillin derivative, cyclization of the substituted vanillin to form a phenylcoumaran, and extension of the aldehyde side chain. Thus, II [R2 = ido, -R3 = CHGMe)2], was treated with BULi and DMF followed by reaction with MeSCH2SOMe and methanolysis to give II (R2 = CH2COZMe, R3 = CH(CMe)2, III). III was condensed with II (R2 = H, R3 = CR0) in the presence of LiN(CDMe2) to give 80% threo-IV (R4 = COZMe). Subsequent silylation and reduction gave field IV (R4 = CHZOH). The diol was then hydrogenated and cyclized by treating with Et20.BF3 in CHCI2. A Wittig reaction of the resulting phenylcoumaran V with 1,3-dioxan-2-ylmethyltriphenylphosphonium bromide followed by NaBH4 reduction gave I (R = H, R1 = CMe) in 90% overall yield.
73022-32-99
RL: RCT (Reactant): SFN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation and reduction of)
73022-32-9 CAPUS
Benzenepropanoic acid, o-[5-(dimethoxymethyl)-3-methoxy-2-(phenylmethoxylphenyll-3-methoyl-4-(phenylmethoxyl)-B[{trimethylsilyloxy}-, methyl ester, (R*,5*)- (9CI) (CA INDEX NAME)

ANSWER 103 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN Relative stereochemistry.

73022-30-7P 73022-30-7P
RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and silylation of)
73022-30-7 CAPLUS
Benzenepropanoic acid, a-[5-(dimethoxymethyl)-3-methoxy-2-(phenylmethoxy)phenyl]-β-hydroxy-3-methoxy-4-(phenylmethoxy), methyl ester, (R*,S*)- (9C1) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 104 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN ester (9CI) (CA INDEX NAME)

ANSWER 104 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1979:473877 CAPLUS 91:73877 91:11933a,11936a Bimolecular self-reactions of 2-arylindandion-1,3-yl radicals studied by flash photolysis Khudyakov, I. V.; Yasmenko, A. I.; Kuz'min, V. A. Inst. Chem. Phys., Moscow, 117334, USSR International Journal of Chemical Kinetics (1979), 11(6), 621-33 CODEN: JUCKBO; ISSN: 0538-8066 Journal English AU CS SO

Kinetic and thermodn. data for the title reaction of aromatic radicals I [R Kinetic and thermodn. data for the title reaction of aromatic radicals I {R H, R1 = NMe2 (II), R = H,R1 = NEt2 (III), R = H,R1 = NPr2 (IV), R = H, R1 = NPr2 (IV), R = H, R1 = NPr2 (IV), R = H, R1 = NPr2 (VII), R = R, R1 = NPr2 (VIII), IX, X, and XI were obtained. The recombination reactions involving radicals II-V are limited by diffusion in solvents having a viscosity ny 10cP and are activation reactions in solvents having a viscosity ny 10cP and are activation reactions in solvents having a viscosity ny 10cP. The recombination of radicals IX and X is an activation reaction, while that of radicals VI-VIII is diffusion-controlled in the entire viscosity range. The recombination of radicals XI is limited, in the viscosity range of 10.4 to 2 ct, by intrusion into the first coordination sphere of the partner, the effect of viscosity on the radical XI recombination rate in the specified range being the same as its effect on diffusion-controlled reactions. The possible reasons of the discrepancies between the exptl. fast recombination rate consts. and the theor. values calculated by the Debye-Smoluchowski theory are discussed. The equilibrium constant depends strongly on the nature of the substituent in the Ph fragment: the substituents which increase unpasied electron delocalization in the radical intensify the dissociation of the resp. dimer.

RL: PROC (Process) (dissociation of) 11023-19-3 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2,4,6-trimethylphenyl)-, diethyl

L4 ANSWER 105 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

N 1979:419465 CAPLUS
DN 91:19465 CAPLUS
DN 91:19465 CAPLUS
COREF 91:3249a, 2252a
TI Voltammetric study of the anodic oxidation of enolate carbanions
AU Kern, Jean Marc: Federlin, Paul
CS Inst. Chim., Univ. Louis Pasteur, Strasbourg, 67000, Fr.
SO Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1978), 96(2), 209-28
CODEN: JEIEBC: ISSN: 0022-0728
DT Journal
LA English
AB A voltammetric study of the anodic oxidation of the enolate carbanions of B-ketonitriles RCH(CN)COR1 has been carried out in Me250. The variation of Eos of these species as a function of the nature of R and RI was examined Their anodic oxidation process could be identified by anal. the voltampercometric curves obtained both at the rotated Pt electrode and at the stationary electrode. Cyclic voltammetry has confirmed that this is an ec overall irreversible process. The electrochem: reaction e yielding a neutral radical is followed by the very fast dimerization (2nd-order chemical reaction c). The fornation of different kinds of dimers, depending on the nature of the oxidized enolates, has been observed during depending on the nature of the oxidized enolates, has been observed during

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PRINTOUT

L4 ANSVER 106 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1979:203702 CAPLUS 90:203702 OREF 90:23393a, 32396a TI 5-Oxopentanoic acid derivatives IN Fisnerova, Ludmila; Nemero Czech. 50 Czech. 6 5-Oxopentanoic acid derivatives Fisnerova, Ludmila: Nemecek, Oldrich: Grimova, Jaroslava IN Fisnerova, Lu PA Czech. SO Czech., 6 pp. CODEN: CZXXA9 DT Patent LA Czech FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE PI CS 176744 PRAI CS 1975-2824 GI CS 1975-2824 19750423 B1 A 19770630

The title compds. I (R1 = H, C3-4 alkyl, Cl, NO2, OMe: R2 = H, CHMe2, NMe2, Cl, NO2: R3 = Ph, 2-furyl, OMe3, 3-indanyl, C6H3C12-2,4) were prepared by addition of 4-R1C6H4CH2CO2Et to 4-R2C6H4CH:CHCOR3 and saponification of

product. Thus, a solution of 2.46 g PhCH2CO2Et and 3.7 g
4-Me2CHCGH4CH:CHCOPh in Et2O containing EtONa was kept 5 days to give 4.4 g
PhCOCH2CH(CGH4CH62-4)CHPhCO2Et which was refluxed with AcOH-HBr to yield
3.5 g I (R1 = H, R2 = CHM2C, R3 = Ph). Similarly prepared were
PhCOCH2CH4CH8CO2H (R4 = 2-pyrrolyl, 3-pyridyl; R5 = Ph, CGH4NO2-4,
CGH4CH2CH4CH8CO2H (R4 = 2-pyrrolyl, 3-pyridyl; R5 = Ph, CGH4NO2-4,
S9771-47-0P 70334-43-9P 70334-45-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
59771-47-0 CAPLUS
Benzenepentanoic acid, B-[4-(1-methylethyl)phenyl]-a-[4-(1-methylropyl)phenyl]-8-oxo-, ethyl ester (9CI) (CA INDEX NAME)

.vz.vu-q.-z LAPLUS Butanedicic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, 1,4-diethyl ester (CA INDEX NAME)

70245-03-3 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, ethyl methyl ester (9CT) (CA INDEX NAME)

ANSWER 106 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

70334-43-9 CAPLUS

Benzenepropanoic acid, \$\textit{\beta} - (3, 3-\text{dimethyl-2-oxobutyl}) - 4-(1-\text{methylethyl}) - a-[4-(2-\text{methylpropyl}) phenyl]-, ethyl ester (CA INDEX NAME)

70334-45-1 CAPLUS Benzenepropanoic acid, β -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- α -[4-(1-methylethyl)phenyl]-, ethyl ester (CA INDEX NAME)

ANSWER 107 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

70245-07-7 CAPLUS
Butanedicia caid, 2,3-dicyano-2-[4-methyl-2-[(methylthio)methyl]phenyl]-3(4-methylphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)

70245-08-8 CAPLUS

SETUDO BULTANCIO SCI, 2,3-dicyano-2-[4-methyl-2-[(methylthio)methyl]phenyl]-3-[4-methyl-3-[(methylthio)methyl]phenyl]-, dimethyl ester (9CI) (CA INDEX NAME)

L4 ANSYER 108 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1979:138070 CAPLUS
DN 90:138070
OREF 90:21905a,21908a
TI The structure of the spermine alkaloid aphelandrine from Aphelandra The structure of the spermine aixaloid appelanding from appelanding squarross Nees
Daetwyler, Peter: Bosshardt, Herbert; Bernhard, Heinz O.; Hesse, Manfred;
Johne, Siegfried
Org.-Chem. Instr., Univ. Zurich, Zurich, Switz.
Helvetica Chimica Acta (1978), 61(7), 2646-71
CODEN: HCACAV; ISSN: 0018-019X ΑU DT LA GI

٠ί.

The structure of aphelandrine from A. squarrosa was determined to be I from chemical and spectral data.
69721-65-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
69721-65-9 CAPLUS
Benzenepropanoic acid, a-[2-hydroxy-5-(3-methoxy-3-oxopropyl)phenyl]4-methoxy-, methyl ester (CA INDEX NAME)

ANSWER 109 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 109 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1979:103658 CAPLUS 90:103658 90:103658 90:16363a,16366a Substituted phenylacetonitrile Maurer, Manfred; Lange, Fritz Walter: Orth, Winfried; Miele, Heinrich; Fickert, Werner Ruetgerswerke A.-G., Fed. Rep. Ger. Ger. Offen., Z6 pp. CODEN: GWXXEX Patent DT Patent LA German FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE PI DE 2708142 DE 2708142 DE 2708142 ES 462366 CH 632236 FR 2381750 PRAI DE 1977-2708142 19780831 19770225 A1 B2 C3 DE 1977-2708142 19800918 19811029 19780601 ES 1977-462366 CH 1977-15344 FR 1978-4716 19770914 19820930 19771213 19780220 19780922 19770225 MARPAT 90:103658

Substituted phenylacetonitriles I (R.= Cl-4 alkyl, C5-7 cycloalkyl or benzyl, optionally substituted by Br, Cl or carbalkoxy: Rl and R2 = Cl-4 alkyl) and 3-H02CCGH4CHRCN (II, R = same as in I) were prepared Thus, 3-Me02CCGH4CH2Cl reated successively with NaCN, Na and Me0COZMe gave 3-Me02CGH4CNa(CN)COZMe which, treated with Me2SO4 gave I (R = R1 = R2 = Me), which was saponified and partially decarboxylated to give II (R = Me). 68433-08-9P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, saponification and partial decarboxylation of) 68433-08-9 CAPLUS Benzenepropanoic acid, 4-chloro-q-cyano-q-[3-(ethoxycarbonyl)phenyl]-, ethyl ester (CA INDEX NAME) ΙT

L4 ANSWER 111 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1979:6107 CAPLUS
DN 90:6107
OREF 90:1109a,1112a
T1 3-Carboxyphenylacetic acid derivatives
IN Maurer, Manfred; Lange, Fritz Walter; Orth, Winfried; Miele, Heinrich; Fickert, Werner
PA Ruetgerswerke A.-G., Fed. Rep. Ger.
Ger. Offen., 25 pp.
CODEN: GWXXEX
DT Patent
LA German
FANLCHT 1

FAN.	CNT 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PΙ	DE 2708143	A1	19780831	DE 1977-2708143	19770225
	DE 2708143	B2	19800626		
	DE 2708143	C3	19811119		
	NL 7713112	A	19780829	NL 1977-13112	19771129
	ES 464851	A1	19780801	ES 1977-464851	19771207
	AT 7801340	A	19790515	AT 1978-1340	19780224
	AT 353777	В	19791210		
	GB 1555849	A	19791114	GB 1978-7732	19780227
PRA	I DE 1977-2708143	A	19770225		

DE 1977-2708143 A 19770225
3-HOZCCGH4CHRCO2H (I, R = Cl-4-alkyl, C5-7-cycloalkyl, benzyl or substituted benzyl) were prepared in 5 steps from alkyl a-chlorom-toluates. Thus, 3-CICH2CGH4CO2Et successively treated with NaCN and Na-E12CO3 gave 3-EtO2CCGH4CNa(CN)COZEt, which was methylated, partially decarboxylated and hydrolyzed to give I (R = Me).
68433-08-9P

68433-08-9P
RL: SPM (Synthetic preparation); PREP (Preparation)
(preparation and partial decarboxylation and hydrolysis of)
68433-08-9 CAPLUS

68433-08-9 CAPLUS Benzenepropanoic acid, 4-chloro-α-cyano-α-[3-(ethoxycarbonyl)phenyl]-, ethyl ester (CA INDEX NAME)

ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

59667-04-8 CAPLUS Benzenepropanoic acid, 2,6-dichloro-α-(4-chlorophenyl)-, ethyl ester (CA INDEX NAME)

59667-13-9 CAPLUS Benzenepropanoic acid, 2,4-dichloro- α -{2,6-dichlorophenyl}-, methyl ester (CA INDEX NAME)

59667-14-0 CAPLUS Benzenepropanoic acid, 4-chloro-q-(2,6-dichlorophenyl)-, methyl ester (CA INDEX NAME)

59667-36-6 CAPLUS Benzenepropanoic acid, 4-chloro- α -(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

L4 ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1977:601405 CAPLUS DN 87:201405 CAPLUS COPYRIGHT 2007 ACS on STN Antimycotic imid-87:31887a,31890a
Antimycotic imidazoles. 2. Synthesis and antimycotic properties of l-[2-(arylalkyl)-2-phenylethyl]-1H-imidazoles
Heeres, Jan; Hostmans, Jozef H.; Van Cutsee, Jan
Res. Lab., Janssen Pharm., Beerse. Belg.
Journal of Medicinal Chemistry (1977), 20(11), 1511-16
CODEN: JMCMAR; ISSN: 0022-2623
Journal
English
CASREACT 87:201405

1-[2-(Arylalkyl)-2-phenylethyl]-1H-imidazoles I (Rn = 2-Cl, -Br, -Me, 4-Cl, 2,4-, 2,6-Cl2; Rln = H, 2-, 4-Cl, 4-Br, -OMe, 2,4-, 2,6-Cl2; m = 1, 2) were prepared from the corresponding RnCGH5-nCH2CN via successive alkylation with X(CH2)mCGH5-nRh1 (X = halo), conversion to the corresponding ester RnCGH5-nCH(CO2N) (CH2)mCGH5-nRh1 (R = Me, Et), and NaBH4-Lil reduction to RnCGH5-nCH(CH2NH) (CH2)mCGH5-nRh1. These alcs. were mesylated and the products refluxed with imidazole in DMF to yield I which were active in vitro against dermatophytes, yeasts, other fungi, and gram-positive bacteria. Some were also active in vivo against Candida albicans.

gram-positive bacteria. Some were also active in vivo against Candida albicans.
59667-03-TP 59667-04-8P 59667-13-9P
59667-14-0P 59667-36-6P 59667-38-8P
64008-30-6P 64008-31-7P 64008-32-8P
64008-33-9P 64008-34-0P 64008-35-1P
64008-39-5P 64008-37-3P 64008-38-4P
64008-39-5P 64008-40-8P 64008-41-9P
64008-42-0P 64008-44-2P'
RL: RCT (Reactant) SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
59667-03-7 CAPLUS
Benzenepropanoic acid, 2,4-dichloro-q-(2-chlorophenyl)-, methyl

Benzenepropanoic acid, 2,4-dichloro-q-(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

59667-38-8 CAPLUS Benzenepropanoic acid, 2,6-dichloro- α -(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

64008-30-6 CAPLUS Benzenepropanoic acid, 2,4-dichloro-α-(2-methylphenyl) ~, methyl ester (CA INDEX NAME)

64008-31-7 CAPLUS
Benzenepropanoic acid, 2,6-dichloro-α-(2-methylphenyl)-, methyl
ester (CA INDEX NAME)

64008-32-8 CAPLUS Benzenepropanoic acid, 4-chloro-a-{2-methylphenyl}-, methyl ester (CA INDEX NAME)

ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

64008-33-9 CAPLUS Benzenepropanoic acid, 2-chloro-a-(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

64008-34-0 CAPLUS Benzenepropanoic acid, q-(2-bromophenyl)-2,4-dichloro-, methyl ester (CA INDEX NAME)

64008-35-1 CAPLUS Benzenepropanoic acid, q-(2-bromophenyl)-4-chloro-, methyl ester (CA INDEX NAME)

64008-36-2 CAPLUS Benzenepropanoic acid, 2-chloro- α -(4-chlorophenyl)-, ethyl ester (CA INDEX NAME)

ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

64008-41-9 CAPLUS Benzenepropanoic acid, 2,6-dichloro- α -{2,4-dichloropheny1}-, ethylester (CA INDEX NAME)

64008-42-0 CAPLUS Benzenepropanoic acid, 4-bromo- α -(2,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)

64008-44-2 CAPLUS Benzenepropanoic acid, q-(2,4-dichlorophenyl)-4-methoxy-, methyl ester (CA INDEX NAME)

ANSWER 112 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Benzenepropanoic acid, 2,4-dichloro-a-(4-chlorophenyl)-, ethyl ester (CA INDEX NAME)

64008-38-4 CAPLUS Benzenepropanoic acid, 2-chloro-a-(2,4-dichlorophenyl)-, methyl ester (CA INDEX NAME)

64008-39-5 CAPLUS Benzenepropanoic acid, 4-chloro-q-(2,4-dichlorophenyl)-, ethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\$$

64008-40-8 CAPLUS Benzenepropanoic acid, 2,4-dichloro- α -(2,4-dichloropheny1)-, ethyl ester (CA INDEX NAME)

L4 ANSWER 113 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1977:72650 CAPLUS DN 86:72650 OREF 86:11519a,11522a Tl 1-(P-A-YJ-P-R-ethyl)imidazoles as antimicrobial agents IN Heeres, Jan: Backx, Leo J. J.: Mostmans, Joseph H. A Janssen Pharmaceutica N. V., Belg. U.S., 18 pp. Division of U.S. 3,927,017. COODE: USXXAM Patent

LA FAN	English .CNT 2				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE.
PI	US 3991201	Α	19761109	US 1975-578777	19750519
	US 3927017	A	19751216	US 1974-483587	19740627
PRA:	I US 1974-483587	A3	19740627		

Arylethylimidazoles I (R = 4-FC6H4, 4-C1C6H4, 2-C1C6H4, 2,4-C12C6H3, 2,6-C12C6H3, Ph; R1 = C1-8 alkyl, allyl, 2-C1C6H4CH:CHCH2, chlorobenzyl, bromobenzyl, cyclohexyl, cyclopentyl, 4-HeCC6H4CH2, 4-HeCGH4CH2) (55 compds.) were prepared by treating RCH2CN with R1Br, hydrolyzing RRICHCN, esterifying RRICHCO2H, LiRH4 reduction of RRICHCO2He, treatment of MCH2CH4 RR1CHCH20H

HCH2OH
with MeSO3H, and treatment of RRICHCH2O3SMe with imidazole.
59667-13-9P
REL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)
(preparation and reduction of)
59667-13-9 CAPLWS

Benzenepropanoic acid, 2,4-dichloro-a-(2,6-dichlorophenyl)-, methyl ester (CA INDEX NAME)

ΙT

59667-03-7P 59667-04-8P 59667-14-0P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 59667-03-7 CAPUS Benzenepropanoic acid, 2,4-dichloro-a-(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

ANSWER 113 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

59667-04-8 CAPLUS
Benzenepropanoic acid, 2,6-dichloro-e-(4-chlorophenyl)-, ethyl ester
(CA INDEX NAME)

59667-14-0 CAPLUS

Benzenepropanoic acid, 4-chloro- α -(2,6-dichlorophenyl)-, methyl ester (CA INDEX NAME)

L4 ANSWER 115 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1976:446150 CAPLUS
DN 85:46150
RF 85:7487a, 7490a
TI The erythro and threo isomers of 2,3,4-substituted butanoic acids
AU Fisnerova, L., Kakac, B.; Kraus, E.; Nemecek, O.
CS Res. Inst. Pharm. Biochem., Prague, Czech.
COCOLECTION OF Czechoslovak Chemical Communications (1976), 41(2), 623-32
CODEN: CCCCAK; ISSN: 0010-0765

Journal English CASREACT 85:46150

DT LA OS GI

Title compds. I (R = Ph, Me3C; Rl = Ph, 4-Me2NCGH4, 4-Me2CHCGH4, 4-ClCGH4, 4-OlNCGH4, 3-pyridyl, 4-Me0CGH4, 2-pyrrolyl; R2 = H, NO2, Me2CHCH2, EtCHMe, Me2CH, Cl, MeO; R3 = H, E1) were prepared and tested for antiinflammatory activity. I were prepared by reaction of ROCCH:CHR1 and p-R2CGHCH2CO2R3 catalyzed by NaNH2 in NH3 (l) for R3 = H and by EtONa in Et2O for R3 = Et. Some I (R3 = H) were prepared by hydrolysis of the corresponding I (R3 = Et) in boiling AcOH-HBT. The three isomers were obtained by the NaNH2-NH3(l) method or by epimerization of the erythro isomers via enol lactones. The highest antiinflammatory activity was found in I (R = Ph, R1 = 3-pyridyl, R2 = Ne2CHCH2, R3 = H) and I (R = Ph, R1 = 4-Me2CHGH4, R2 = R3 = H) (II). The effect of configuration on the antiinflammatory activity was also studied: three-II was .apprx.15% more active than erythro-II.

59771-64-D9 55771-64-1P 59771-65-2P
59771-10-D9 59771-66-F 59771-70-9P
59771-71-DP

59771-71-0P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation and hydrolysis of)
59771-47-0 CAPLUS
Benzenepentanoic acid, %-[4-{]-methylethyl]phenyl]-a-[4-{]-methylpropyl)phenyl]-8-0xo-, ethyl ester (9CI) (CA INDEX NAME)

59771-64-1 CAPLUS
Benzenepentanoic acid, α,β-bis[4-(1-methylethyl)phenyl]-δ-oxo-, ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

L4 ANSWER 115 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Relative stereochemistry.

59771-65-2 CAPLUS

Senzenepentanoic acid, α,β-bis[4-(1-methylethyl)phenyl]-δ-oxo-, ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

59771-68-5 CAPLUS
Benzenepropanoic acid, β-(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)α-[4-(2-methylpropyl)phenyl}-, ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

59771-69-6 CAPLUS Benzenepropanoic acid, β -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- α -(4-(2-methylpropyl)phenyl]-, ethyl ester, {R*,5*}- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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ANSWER 115 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

59771-70-9 CAPLUS Benzenepropanoic acid, β-{3,3-dimethyl-2-oxobutyl}-4-(1-methylethyl)-a-[4-(1-methylethyl)phenyl]-, ethyl ester, (R*,R*)- (9CI) (CA INDEX

Relative stereochemistry.

$$\begin{array}{c} \mathbf{i}\text{-Pr} \\ \\ \mathbf{b} \\ \\ \mathbf{r} \\ \\$$

59771-71-0 CAPLUS Benzenepropanoic acid, β -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- α -[4-(1-methylethyl)phenyl]-, ethyl ester, (R*,S*)- (9CI) (CA INDEX

Relative stereochemistry.

ANSWER 116 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Contisted Contisted Cont

59667-04-8 CAPLUS Benzenepropandic acid, 2,6-dichloro- α -(4-chlorophenyl)-, ethyl ester (CA INDEX NAME)

59667-14-0 CAPLUS
Benzenepropanoic acid, 4-chloro-q-(2,6-dichlorophenyl)-, methyl
ester (CA INDEX NAME)

ΙŤ

59667-36-6 59667-37-7 59667-38-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
59667-36-6 CAPUS
Benzenepropanoic acid, 4-chloro-a-(2-chlorophenyl)-, methyl ester
(CA INDEX NAME)

59667-37-7 CAPWS

L4 ANSWER 116 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN N 1976:433007 CAPLUS N 85:33007 CAPLUS N 85:33007 CAPLUS N 19:3007 N 19 DT Patent LA English FAN.CNT 2 PATENT NO. KIND APPLICATION NO. DATE DATE PI US 3927017 US 3991201 PRAI US 1974-483587 GI 19751216 19761109 19740627 19750519 US 1974-483587 US 1975-578777

Imidazoles I [Rn = Cl, F, H, 2,4-, 2,6-Cl2: Rl = alkyl, allyl, cycloalkyl, CH2CGH5R2,CH2CGH4Cl2-2,4, CH2CGH4Cl2-2,6: R2 = Cl, Br, 4-Me, 4-MeO, CH2CH2Ph] (SJ compds.), fungicides, bacteriostats, and bactericides at 0.1-100 y/ml, were prepared by treating benzeneacetonitriles II (R3 = H) with halides RIX, hydrolyzing-esterifying II (R3 = R1) with HCl in MeOH or EtOH, reducing the ester RnCGH5-nCHR1CQ2A4 (R4 = Me, Et) with NaBH4 over LiX in MeCN, mesylating the alc. RnCGH5-nCHR1CH2OH, and treating the methanesulfonate with imidazole.

59667-13-99

59667-13-9P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reduction of) 59667-13-9 CAPLUS Benzenepropanoic acid, 2,4-dichloro- α -(2,6-dichlorophenyl)-, methyl ester (CA INDEX NAME)

59667-03-7P 59667-04-8P 59667-14-0P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) ΙT

ANSWER 116 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Benzenepropanoic acid, 2-bromo-d-(2,4-dichlorophenyl)-, methyl estet (CA INDEX NAME)

59667-38-8 CAPLUS Benzenepropanoic acid, 2,6-dichloro-α-(2-chlorophenyl)-, methyl ester (CA INDEX NAME)

L4 ANSWER 117 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1974:42619 CAPLUS
DN 81:26419
OREF 81:42653,4268a
T1 Testing procedure for catalysts in polyester moldings
AS Simmonds, John: Roskott, L.
CS Novadel Ltd., Gillingham/Kent, UK
Proceedings of the Annual Conference - Reinforced Plastics/Composites
Institute, Society of the Plastics Industry (1973), 28, 1C, 12 pp.
CODEN: PCRPBG: ISSN: 0160-9750
DT Journal
LA English
AB The most useful tests were determination of the time to peak exotherm of pure

pure polyester and of molding compound and determination of shrinkage as measured by a displacement meter, which indicated min. molding time, and the kick-off time (where the kick-off temperature showed a marked diversion from the warming-up curve, which was a measure of gel time. Also valuable were residual styrene [100-42-5] determination, indicating degree of curing, and

Warming-up curve, which can be residual styrene [100-42-5] determination, indicating degree of curing, and gloss determination by a gloss meter (DIM 67530), the main parameter by which the appearance of the product was judged. Four different peroxide types, i.e., benzoyl peroxide [9-4-36-0], tert-butyl peroxide [9-2-thyl hexanoate [3006-82-4], 1,1-bis(tert-butyl peroxy)-3,3,5-trimethylcyclohexane [6731-36-8], and (m-phenylene disopropylidene)bis[tert-butyl peroxide] [2212-91-9] were used as initiators, and the test methods also predicted the performance of a bibenzyl or G-C initiator, 1,2-bis(p-methylphenyl)-1,2-dimethoxycarbonyl-1,2-dicyanoethane [31249-03-3].

II 31249-03-3
RL: CAT (Catalyst use); USES (Uses) (catalyst, for crosslinking of unsatd. polyester molding compound, evaluation of)

RN 31249-03-3 CAPLUS
CN Butanediolc acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester (9C1) (CA INDEX NAME)

DN 80:84002 CAPI
N 80:84002 CAPI
N 80:84002
OREF 80:13533a,13536a
TI Evaluating catalv
AU Simmonds, J.
CS Novadel
SO Mrd ANSWER 119 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1974:84002 CAPLUS SUIISSIA, 13536A
SYMMOTON CATALOGUE FOR PROPERTY OF THE PROPER English English
Improved gloss and stability were imparted to polyester molding compds, by replacement of diacyl, perketal, peroxy ester, or dialkyl peroxide catalysts with 1,2-bis/pe-methylphenyl)-1,2-dicarbomethoxy-1,2-dicyanoethane [31249-03-3].
31249-03-3
RL: USES (Uses)
(catalysts for crosslinking of unsatd. polyesters)
31249-03-3 CAPIUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester (9CI) (CA INDEX NAME) ΙT

ANSWER 118 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1974:133668 CAPLUS 80:133668 30:133668
30:133668
90:21361a,21564a
Photosensitized oxidation of an enaminoketone. Total synthesis of a rhoeadine alkaloid
Orito, K.; Manske, R. H.; Rodrigo, R.
Dep. Chem., Univ. Waterloo, Waterloo, ON, Can.
Journal of the American Chemical Society (1974), 96(6), 1944-5
CODEN: JACSAT; ISSN: 0002-7863
Journal
English
For diagram(s), see printed CA Issue.
(i) cis-Alpinine I was synthesized. Indenone intermediate II, prepared by standard methods was oxidatively rearranged in a dye-sensitized photo-oxidation process to ketolactone III which was transformed into 1.
52658-50-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
52658-50-1 CAPUS
Benzenepropanoic acid, α-[2-(2-(acetylmethylamino)ethyl)-4,5-dimethoxyphenyl]-2,3-dimethoxy-, ethyl ester (CA INDEX NAME) OREF 80:21561a,21564a TI Photosensitized

L4 ANSWER 120 OF 1 AN 1974:59616 CAI DN 80:59616 OREF 80:9665a,9668a TI Chemical struct ANSWER 120 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1974:59616 CAPLUS 80:59616

Chemical structure and sweet taste of isocoumarins and their derivatives.

IV Yamato, Masatoshi; Sato, Koichi; Hashigaki, Kuniko; Ishikawa, Tadataka; Koyama, Takaji Med. Sch., Univ. Okayama, Okayama, Japan Yakuyaku Zashi (1973), 93(12), 1639-42 CODEN: YKKZAJ; ISSN: 0031-6903 ΑU

CS SO

CODEN: YKKZAJ; ISSN: 0031-6903
Journal
Japanese
For diagram(s), see printed CA Issue.
Further investigation was made on the derivs. of β-[3-hydroxy-4methoxyphenyl]ethylbenzene which is regarded as the essential structure
for the sweet taste of phyllodulcin, and compds. (I-XII) were synthesized.
Both VIII and XI were sweet, whereas II, III, and IV were tasteless, and
V, VI, VII, IX, X, and XII revealed a bitter taste. On the basis of these
data, a delicate relation between the mol. structure and sweet taste
receptor site was presumed.
51458-16-3P
RLI SPN (Synthetic preparation): PREP (Preparation)

S1438-16-37
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
51458-16-3 CAPLUS
Benzenepropanoic acid, α-[2-(ethoxycarbonyl)phenyl]-3-hydroxy-4-methoxy-, ethyl ester (CA INDEX NAME)

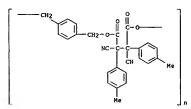
L4 ANSWER 121 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1973:515413 CAPLUS
N 79:115413
OREF 79:18743a, 18746a

TI Reactions of the 2-(1H)-pyridinones prepared from 4,4-dimethoxychalcone and anisal acetone
AU Samour, A.; Fahmy, A. Farouk: Abd El-Rahman, S.; Akhnookh, Y.; Abd El-moez, M. S.
CS Fac. Sci., Ain Shams Univ., Cairo, Egypt
United Arab Republic Journal of Chemistry (1971), 14(6), 581-98
CODEN: UAACAZ: ISSN: 0372-3704
U Journal
LA English
GF For diagram(s), see printed CA Issue.
AB RCOCH:CHCGH4OMe-p undervent cycloaddn. with NCCH2CO2Et to give the pyridines I (R = Me, p-MeOCH4) and the nicotinoates II (R = Me, p-MeOCH4). MeCOCH:CHCGH4OMe-p and NCCH2CN gave the nicotinate III. I was treated with Grignard reagents, PCC13, and its potassium salt alkylated: e.g. I (R = Me) and PhMgBr gave the pyridone IV.
T 50548-86-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50548-86-2 CAPLUS
CN Benzenepentanoic acid, α-(4-chlorophenyl)-4-methoxy-β-(4-methoxy

L4 ANSWER 122 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 122 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1973:111801 CAPLUS
N 78:111801
OREF 78:17963a,17966a
T1 Oxidative carbon-carbon coupling. III. Oxidative polymerization of bifunctional arylcyanoacetic esters
AU De Jongh, H. A. P.; De Jonge, C. R. H. I.; Sinnige, H. J. M.; Magre, E. P.; Mijs, V. J.
CS Corp. Res. Dep., Akzo Res. Lab., Arnhem, Neth.
SJ Journal of Polymer Science, Polymer Chemistry Edition (1973), 11(2), 345-52
CODEN: JPLCAT; ISSN: 0449-296X
DT Journal
LA English
AB Bifunctional arylcyanoacetic esters were oxidatively coupled to give high mol. weight, colorless, amorphous polymers, soluble in common organic solvents.
Brittle films were obtained by casting or compression molding. Thermal stability of the polymer was poor due to the weak C-C bond formed by oxidative coupling. Radical dissociation-recombination of this bond resulted in meso-dl equilibration, lowering the glass transition temperature of the polymers.

IT 41072-40-6 d1072-41-7
RL: PRP (Properties)
[Solution and thermal properties of)
RN 41072-40-6 CAPLUS
NAME)



RN 41072-41-7 CAPLUS
CN Poly[oxy[2,3-dicyano-2,3-bis(4-methylphenyl)-1,4-dioxo-1,4-butanediyl]oxymethylene-1,4-cyclohexanediylmethylene] (9CI) (CA INDEX NAME)

L4 ANSWER 123 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1972:552898 CAPLUS DN 77:152898 OREF 77:25147a, 25150a Aradical-initiated chemical reactions Akzo N. V. Neth. Appl., 8 pp. CODEN: NAXXAN DT Pate LA Dutc FAN.CNT 1 Patent Dutch PATENT NO. KIND DATE APPLICATION NO. DATE NL 7205982 19720725 NL 1972-5982 19720503 NL 7205982 19/20/25 NL 19/2-3902 19/20005 Three I and five II were used as radical polymerization initiators for AB Three I and five II were used as radius; polymerically in the styrene [100-42-5] or Me methacrylate (III) [80-62-6] at 80-120.deg.; 24-98t yields were obtained. In addition II [RI = p-xylylene, R2 = Me, Y = O, n = 190) (IV) was a stabilizer for III <40.deg.. In an example, 25 ml styrene and 56.8 mg IV was kept 2 hr at 120.deg. to give 56 polystyrene [9003-53-6] as compared to 34t for tert-Bu202 initiator. The I had R = Me, Bu, or n-decyl with m = 40-60; other II had R1 = 1,4-dimethyleroclohutylene; R2 = Me, or tert-octyl; Y = O or MH; and n = 85-190. 85-190. 38807-91-9 41072-40-6 41072-41-7 IT

RN 41072-40-6 CAPLUS

CN Poly[cxy[2], 3-dicyano-2, 3-bis (4-methylphenyl)-1, 4-dioxo-1, 4-butanediyljoxyethylene-1, 4-phenylenesthylene) (9CI) (CA INDEX NAME)

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ANSWER 123 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

41072-41-7 CAPLUS
Polylomy[2,3-dicyano-2,3-bis(4-methylphenyl)-1,4-dioxo-1,4-butanediyl]oxymethylene-1,4-cyclohexanediylmethylene| (9CI) (CA INDEX NAME)

L4 ANSWER 124 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Relative stereochemistry.

30698-39-6 CAPLUS Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, dimethyl ester, (%',5')- (9CI) (CA INDEX NAME)

Relative stereochemistry.

30698-40-9 CAPLUS
Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, dimethyl ester, [R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

34404-72-3 CAPLUS 1,1.2,2-Ethanetetracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetramethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 124 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1972:502330 CAPLUS DN 77:102330 COPET 77:16876h, 16877a TI Radical initiation of vinyl polymerization by //:10230/
//:10230/
//: Radical initiation of vinyl polymerization by
a,a,a',a'-a'-tetrasubstituted dibenzyls
De Jongh, H. A. P., De Jonge, C. R. H. I., Huysmans, W. G. B.; Sinnige, H. J. M.; De Klein, W. J.; Mijs, W. J.; Jaspers, H.
Akzo Res. Lab., Arnhem, Neth.
Makromolekulare Chemie (1972), 157, 279-98
CODEN: MACEAK: ISSN: 0025-116X
Journal
English
The polymerization reactivity of styrene [100-42-5], Me methacrylate
-62-6], and acrylonitrile [107-13-1] in the presence of a,a'dicyanodibenzyls a,a'-disubstituted with ester, nitrile,
amide, or Ph groups in the presence of a,a,a'tetrakis (methoxycarbonyl) dibenzyl [3404-71-2] was higher than that of
vinyl acetate [108-05-4] and vinyl chloride [75-01-4], with the styrene
polymerization rate generally comparable to that in the presence of
oxides and ΑU peroxides and affected by the \(\alpha \) - and ring-substituents and stereochemistry. The meso-\(\alpha \) - \(\alpha \) dicyanodibenzyls \(\alpha \), \(\alpha \) disubstituted with ester groups gave a 2.5-3.5 fold faster polymerization than their DL-isomers.
The dissociation rate consts., determined from NMR line widths, indicated DL-isomers.

The dissociation rate consts., determined from Non Asia.

That the

a,a'-dicyanodibenzyls a,a'-disubstituted with
ester groups were good initiators while those with Ph and nitrile groups
were inefficient. Initiation and termination mechanisms based on
1,2-addition of the dibenzyl catalysts to styrene are given.

IT 30698-37-4 30698-38-5 30698-39-6
30698-40-9 34404-72-3 34404-73-4
34405-32-2 34405-37-3 37760-82-0
37761-19-6 37761-20-9 37761-21-0

RL: CAT (Catalyst use): USES (Uses)
(catalysts, for polymerization of vinyl compds.)

RN 30698-37-4 CAPLUS

CN Butanedicic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester,
(R*,S*)- (9CI) (CA INDEX NAME)

30698-38-5 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester, (R.R.)- (9CI) (CA INDEX NAME)

ANSWER 124 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

34404-73-4 CAPLUS 1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-chlorophenyl)-, tetramethyl ester (9CI) (CA INDEX NAME)

34405-36-2 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2-methylphenyl)-, dimethyl ester, (R^*,R^*) - (9CI) (CA INDEX NAME)

Relative stereochemistry.

34405-37-3 CAPLUS Butanedioic acid, 2,3 ester, (R*,R*)- (9CI) 2,3-dicyano-2,3-bis(2,4-dimethylphenyl)-, dimethyl 9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 124 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

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37760-82-0 CAPLUS Butanedioic acid, 2,3-bis(2-chlorophenyl)-2,3-dicyano-, dimethyl ester, (R,R)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

37761-19-6 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2-methylphenyl)-, dimethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

37761-20-9 CAPLUS
Butanedioic acid, 2,3-bis(3-chlorophenyl)-2,3-dicyano-, dimethyl ester, (R.5+)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 125 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1972:447849 CAPLUS 77:47849

ANSWER 16.3 OF 140 CAPLUS COPYRIGHT 2007 ACS on STN

1972:447849 CAPLUS

N 77:47849

OXIdative carbon-carbon coupling. II. Effect of ring substituents on the oxidative carbon-carbon coupling of arylmalonic esters, arylmalodinitriles, and arylcyanoacetic esters

DE Jongh, H. A. P.; DE Jonge, C. R. H. I.; Sinnige, H. J. M.; DE Klein, W. J.; Waymans, W. G. B.; Mijs, W. J.; Van den Hoek, W. J.; Smidt, J.

CS Corp. Res. Dep., Akzo Res. Lab., Arhhem, Neth.

Journal of Organic Chemistry (1972), 37(12), 1960-6

CODEN: JOCEAH; ISSN: 0022-3263

JOURNAL

LA English

A Arylmalonic esters and arylmalonodinitriles can be coupled oxidatively to the corresponding bibenzyls. Good yields of dimers are obtained when a para substituent (Me. Cl) is introduced, which inhibits the formation of higher oligomers through benzylic C-para C coupling. Substitution at both ortho positions and the para position (Me) in phenylcyanoacetic esters completely inhibits C-C coupling by steric crowding. Keteneimies are formed instead by C-M coupling, Substitution at one ortho position (Me) partially gives the usual C-C coupling together with benzylic C-para C coupling (keteneimine formation) in case of a free para-position and C-N coupling (keteneimine formation) in case of a free para-position and C-N coupling (keteneimine formation) in case of a free para-position are confirmed by ESR anal. Prom NNR line width measurements kinetic parameters for the dissociation reaction are obtained.

IT 3551-80-2

Ripper (Properties)

(ESR of)

J9914-40-2
RL: PRP (Properties)
(ESR of)
39514-80-2 CAPLUS
Butanedioic acid, 2,3-dicyano-2,3-bis(2,4,6-trimethylphenyl)-, dimethyl
ester (9CI) (CA INDEX NAME)

30698-38-5P 34404-72-3P 34404-73-4P 34405-36-2P 34405-37-3P RL: SPN (Synthetic preparation): PREP (Preparation) (preparation of) 30698-38-5 CAPLUS Butanedioc acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 124 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

37761-21-0 CAPLUS Butanedioic acid, 2,3-bis(2-chlorophenyl)-2,3-dicyano-, dimethyl ester, (Rr.5')- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 125 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

34404-72-3 CAPLUS
1,1,2,2-Ethanetatracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetramethyl ester (9CI) (CA INDEX NAME)

34404-73-4 CAPLUS 1,1,2,2-Ethanetetracarboxylic acid, 1,2-bis(4-chlorophenyl)-, tetramethyl ester (9C1) (CA INDEX NAME)

34405-36-2 CAPLUS Butamedidic acid, 2,3-dicyano-2,3-bis(2-methylphenyl)-, dimethyl ester, (R.,R.)- (9C1) (CA INDEX NAME)

ANSWER 125 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

34405-37-3 CAPLUS Butanedioic acid, 2,3-dicyano-2,3-bis(2,4-dimethylphenyl)-, dimethyl ester, (R^*,R^*) - (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 126 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 126 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1972:127800 CAPLUS
ON 76:127800
ORF 76:20591a, 20694a
TI Methyl 1,2-diphenylethanetetracarboxylates as initiators for polymerization of styrene
IN De Jongh, Hendrik A. P.; De Jonge, Cornelis R. H. 1.
AXTO G.m.b.H.
SO Ger. Offen. 14 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

FAN.	CNT 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2132740	A	19720120	DE 1971-2132740	19710701
	DE 2132740	B2	19800703		
	DE 2132740	C3	19810430		
	NL 7009925	Α -	19720105	NL 1970-9925	19700703
•	GB 1336675	A	19731107	GB 1971-30874	19710701
	BE 769414	Al	19711116	BE 1971-105397	19710702
	US 3896099	A	19750722	US 1973-401604	19730928
PRAI	NL 1970-9925	A	19700703		
	US 1971-159949	A2	19710702		

US 19/1-19949 AZ 19/10/02 Tetra-Me 1,2-diphenylethanetetracarboxylate [34404-71-2], tetra-Me 1,2-bis(p-chlorophenyl)ethanetetracarboxylate [34404-73-4], or tetra-Me 1,2-bis(p-tolyl)ethanetetracarboxylate (1) [34404-72-3], prepared by oxidative coupling of the corresponding di-Me arylmalonates with MinO4 or K3FE(GN)6, were used as radical initiators for the

with RMnO4 or K3Fe(CN)6, were used as radical initiators for the
polymerization
of styrene and, in contrast to peroxides or azodinitriles, did not cause
the formation of gaseous products. Thus, 100 ml styrene and 250 mg I were
heated 2 hr at 120.deg, to give 78% polystyrene [9003-53-6] as compared to
34% for tetr-Bu peroxide.
IT 34404-72-3 34404-73-4
RL: CAT (Catalystuse); USES (Uses)
(catalysts, for polymerization of styrene)
RN 34404-72-3 CAPLUS
CN 1,1.2.2-Ethanetetracarboxylic acid, 1,2-bis(4-methylphenyl)-, tetramethyl
ester (9CI) (CA INDEX NAME)

34404-73-4 CAPLUS
1.1,2,2-Ethanetetracarboxylic acid, 1,2-big(4-chlorophenyl)-, tetramethyl ester [9CI] (CA INDEX NAME)

L4 ANSWER 127 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1972:113055 CAPLUS DN 76:113055 CREF 76:18253a,18256a TI Answolytic phenyl-2-pyrrolidinones Strubbe, Josefr Linz, Raymond PA UCB Union Chimique-Chemische Bedrijven S. A. Ger. Offen., 32 pp.

76:18:533,18:508
Anxiolytic phenyl-2-pyrrolidinones
Strubbe, Josef Linz, Raymond
UCB Union Chimique-Chemische Bedrijven S. A.
Gec. Offen., 32 pp.
CODEN: GWXXEX

DT LA

FAN.	CNT 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2136571	A	19720127	DE 1971-2136571	19710722
	DE 2136571	C2	19820325		
	GB 1350582	A	19740418	GB 1970-35948	19700724
	IL 37147	A	19740630	IL 1971-37147	19710624
	NL 7109930	A	19720126	NL 1971-9930	19710719
	FR 2100946	A5	19720324	FR 1971-26784	19710720
	FR 2100946	B1	19750606		
	HU 162344	В	19730129	HU 1971-UI178	19710721
	ES 393496	A1	19730816	ES 1971-393496	19710721
	RO 61127	A1	19761115	RO 1971-67732	19710721
	CS 174822	B2	19770429	CS 1971-5382	19710721
	CS 174849	B2	19770429	CS 1975-6089	19710721
	DK 135584	В	19770523	DK 1971-3580	19710721
	FI 55184	В	19790228	FI 1971-2068	19710721
	FI 55184	С	19790611		
	RO 71354	A1	19820226	RO 1971-81864	19710721
	BE 770308	A1	19720124	BE 1971-3254	19710722
	CA 954870	A1	19740917	CA 1971-118906	19710722
	IN 132195	A1	19750802	IN 1971-132195	19710722
	JP 54017734	В	19790702	JP 1971-54902	19710722
	ZA 7104911	A	19720426	ZA 1971-4911	19710723
	AT 304530	В	19730110	AT 1971-6430	19710723
	AU 7131575	λ	19730125	AU 1971-31575	19710723
	CH 537921	A	19730731	CH 1972-10160	19710723
	CH 538474	λ	19730815	CH 1971-10857	19710723
	AT 310150	В	19730925	AT 1972-1805	19710723
	SU 479293	λ3	19750730	SU 1971-1891416	19710723
	SE 379347	В	19751006	SE 1971-9515	19710723
	SU 488410	A3	19751015	SU 1971-1689301	19710723
	PL 82184	B1	19751031	PL 1971-149583	19710723
	US 3956314	A	19760511	US 1973-417528	19731120
PRAI	GB 1970-35948	λ	19700724		
	US 1971-165342	A2	19710722		
GI	For diagram(s), se	e print	ed CA Issue.		

OS 19/1-103-22 Z 19/10/22
For diagram(s), see printed CA Issue.
Title compds. [I. R = H, alkyl, PhCH2, propynyl, allyl, or cyclopentyl: Rl = H, alkyl, allyl, or (substituted) phenyl: R2 = H or monosubstituted phenyl: R3 = H, Et, Ph, or 2,4-Me2CGH3] were prepared by several methods: cyclization of 4-aninobutyric acids, decarboxylation of 3-carboxy-3-R1-2-pyrrolidinones, or known reactions of phenyl-pyrrolidinones gave ! (R = H) which reacted with NaH and RI to give 1-substituted I. Thus, p-CLGCH4(HCM)-CHPhCO2Et in ETCH was hydrogenated over Raney Ni 15 hr at 90-5 and 100 atm to give .apprx.50% cis-1 (R = R3 = H, R1 = Ph, R2 = 4-p-CLCCH4) (II) and the trans isomer separated by crystallization Similarly prepared were .apprx.45 I, e.g. (R-R3 given): H, 4,4-Me2CG-H3] (III): H, allyl, 3-p-MeCGH4, H; hexyl, Ph, 4-p-CLCGH4, H. Anxiolytic effects were caused by min. doses of 0.0024 mole II/kg rat or

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ANSWER 127 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Co 0.10 mole III/kg rat. 16224-82-59 36263-00-0P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 36224-82-5 CAPLUS Benzenepropanoic acid, 4-chloro-a-(4-chlorophenyl)-\$\beta\$-cyano-, ethyl ester (CA INDEX NAME)

(Continued)

36263-00-0 CAPLUS

Benzenepropanoic acid, 4-chloro-α-(2-chlorophenyl)-β-cyano-, ethyl ester (CA INDEX NAME)

ANSWER 128 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

30698-40-9 CAPLUS
Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, dimethyl ester, (Ry.Ry)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

30698-37-4
RL: PRP (Properties): RCT (Reactant): RACT (Reactant or reagent)
(rearrangement of, kinetics of)
30698-37-4
CAPIUS
Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester,
(R*,5*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 128 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1971:551041 CAPLUS
DN 75:151041
OXIdative carbon-carbon coupling. I. Oxidative coupling of a-substituted benzylcyanides
AU De Jongh, H. A. P.; De Jonge, C. R. H. I.; Mijs, W. J.
CS Corp. Res. Dep., Akzo Res. Lab., Arnhem, Neth.
SO Journal of Organic Chemistry (1971), 36(21), 3160-8
CODEN: JOCEAN; ISSN: 0022-3263
Journal
LA English
GI For diagram(s), see printed CA Issue.
AB OXidative dimerization of benzylcyanides a-substituted with an ester, acyl, or amide group, with a Cu-amine-O system or with other oxidants gave the corresponding 2,3-diphenylsuccinomitriles as a mixture of diastereoisomers in high yields. Configurational assignments are made for dl- and meso-I on the basis of cyclization reactions to give mono or bicyclic succinimides II and III. Thermal equilibration of the dl and meso diastereoisomers takes place in various solvents at 80-150° via radical dissociation-recombination along the central C-C bond. For dimers

(I (Refl. Me) the equilibrium constant X (dl/meso) is 13-16. For the meso

wis radical dissociation-recombination along the central C-C bono. ror dimers

(I (R-H, Me) the equilibrium constant K (dl/meso) is 13-16. For the meso of the conversion of I (R-H, Me), AN is 22-23 kcal/mole and AS is -11 to -12 entropy units. Thermal treatment of the para unsubstituted diester I (R-H) at 130-170° gives redistribution to the monomer PhCH(CN)CO2Me (IV) and oligomers (tri-to pentamers). Similarly, the oxidative coupling of the para unsubstituted benzylcyanides IV, PhCH(CN)Ac, and a (piperidinocarbonyl) benzylcyanide gave rise to various amounts of oligomers. Both oligomerization reactions are impeded by introduction of a para substituent.

IT 30698-38-57 30698-39-67 30698-40-9P

RL: SPN (Synthetic preparation): PREP (Preparation) (preparation of)

RN 30698-38-5 CAPLUS

CN Butanedioic acid, 2,3-dicyano-2,3-bis(4-methylphenyl)-, dimethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

30698-39-6 CAPLUS
Butanedioic acid, 2,3-bis(4-chlorophenyl)-2,3-dicyano-, dimethyl ester, (Rr.51)- (9C1) (CA INDEX NAME)

Relative stereochemistry.

OREF

ANSWER 129 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1971:510166 CAPLUS
75:110166
75:110166
75:17395a,17398a
Isoquinoline-type heterocycles from β-amino acids. II.
Stereospecific syntheses of (+-)-6,7-dialkoxy-3-aryl-4-(methoxycarbonyl)1,2,3,4-tetrahydroisoquinolines and their derivatives
Haimova, Marietta A.; Spassov, Stefan L.; Novkova, Snezana I.; Palamareva,
Mariana D.; Kurtev, Bogdan J.
Fac. Chem., Univ. Sofia, Sofia, Bulg.
Chemische Berichte (1971), 104(8), 2601-10
CODEN: CHEEAN; ISSN: 0009-2940
Journal
German
For diagram(s), see printed CA Issue.

ΑIJ

CS SO

German
For diagram(s), see printed CA Issue.
Me (t)-3-amino-2,3-diarylpropionates gave under the conditions of the
Pictet-Spengler reaction by cyclization stereospecifically in both the
erythro and three series 6,7-dialkowy-3-aryl-4-(methoxycarbonyl)-1,2,3,4tetrahydroisoquinolines [1]. LiAlH4 reduction of I gave the corresponding
4-hydroxymethyl derivs. From the NMR data reported, the conformations of
the compds. are evaluated.
33386-64-0P 33386-65-1P 33386-66-2P
33482-67-6P

33482-67-69
RL: SPN (Synthetic preparation), PREP (Preparation)
(preparation of)
3386-64-0 CAPLUS
β-Alanine, 2-(2-bromo-4,5-dimethoxyphenyl)-3-[2-bromo-4,5-(methylenedioxy)phenyl]-N-formyl-, methyl ester, erythro-(±)- (8CI)
(CA INDEX NAME)

Relative stereochemistry.

33386-65-1 CAPLUS \$\text{B-Alanine}, 2-[2-bromo-4,5-dimethoxyphenyl]-3-[2-bromo-4,5-(methylenedioxy)phenyl]-, methyl ester, erythro-(\darkappa)- (8CI) (CA INDEX NAME)

33386-66-2 CAPLUS

B-Alanine, 2-(2-bromo-4,5-dimethoxyphenyl)-3-[2-bromo-4,5(methylenedioxy)phenyl]-, methyl ester, hydrochloride, erythro-(±)(8C1) (CA INDEX NAME)

Relative stereochemistry.

• HC1

33482-67-6 CAPLUS B-Alanine, 2-(2-bromo-4,5-dimethoxyphenyl)-3-(2-bromo-4,5-(methylenedioxy)phenyl]-N,N-dimethyl-, methyl ester, erythro-(±)- (8CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 130 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1971:88362 CAPLUS
DN 74:88362 .
CREF 74:14349a,1452a
TI * 1.2-Diphenyl-1,2-dicyano-1,2-bis[alkyl (or aryl or amino)peroxy (or oxy) carbonyllethanes as polymerization initiators
IN De Jongh, Hendrik A.; De Jonge, Cornelis R. H. I.
AXZO N. V.
SO GGr. Offen., 18 pp.
CODEN: GWIXEX
DF Patent
LA German
FARM.CNT 1

FAN	.CNT 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	-DATE
PĬ	DE 2033910	λ	19710121	DE 1970-2033910	19700708
	DE 2033910	B2	19810219		
	DE 2033910	C3	19811217		
	NL 6910428	A	19710112	NL 1969-10428	19690708
	NL 161425	С	19800215		
	NL 161425	В	19790917		
	US 3726837	A	19730410	US 1970-52073	19700702
	GB 1270784	A	19720412	GB 1970-1270784	19700707
	BE 753154	A	19701216	BE 1970-753154	19700708
	FR 2054344	A5	19710416	FR 1970-25339	19700708
	AT 300346	В	19720725	AT 1970-6212	19700708
	JP 49045151	В	19741202	JP 1970-59171	19700708
	SE 371011	В	19741202	SE 1970-9465	19700708
PRA	I NL 1969-10428	Α	19690708		

PRAIN NL 1969-10428 A 19690708

AB The reaction-specific, fairly heat-stable compds. of the formula NC(p-R CGH4) [R1(0) noC(c)(C(0)(0) nA]) [CGH4R-p)CN (I), where R = H, Me, Cl., NOZ, or OHe: R1 = Me, Et. Ph, NHZ. NDMe, or pipe ridino, n = 0-1, oxidation resistant, of relatively high activity at lower temps.; inactive at room temperature, and which do not form gaseous products during radical formation are useful as radical initiators for polymerization, e.g., of styrene (II), AcoCH:CHZ, CHZ:CHCN, or CHZ:CMCDMe, or the hardening, e.g., of the unsatd, polyester resin Lupodal P-6. I are prepared by treating the corresponding NC(p-RCGH4)(CH(CO(0)nR1) with O in the presence of CuCl and Me2NCH2CH2NMe2.

IT 31249-03-3 31249-04-4 31249-05-5
R1: CAT (Catalyst use) USES (Uses) (catalysts, for polymerization of vinyl compds.)

RN 31249-03-3 CAPUS

NN 31249-03-3 CAPUS

CM Butanedioic acid, 2,3-dicysno-2,3-bis(4-methylphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)

31249-04-4 CAPLUS Succinic acid, 2,3-dicyano-2,3-di-p-tolyl-, didodecyl ester (8CI) (CA INDEX NAME)

ANSWER 129 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 130 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

31249-05-5 CAPLUS . Succinic acid, 2,3-bis(p-chlorophenyl)-2,3-dicyano-, dimethyl ester (8CI) (CA INDEX NAME)

(Continued)

ANSWER 131 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1969:491021 CAPLUS 71:91021 71:16914h,16915a Non-volatile α-branched chain fatty acid derivatives. IV. Addition of aryl esters to long chain olefins Bilyk, A.; Eisner, A.: Maerker, G. Eastern Util. Res. and Develop. Div., Agr. Res. Serv., Philadelphia, PA, USA JOAN JOURNAL OF THE AMERICAN OIL CHEMISTS' Society (1969), 46(9), 469-72 CODEN: JAOCA7; ISSN: 0003-021X 50 DT LA AB Journal
English
The di-tert-butyl peroxide initiated free radical addition of Me
phenylacetate (1), Me p-tolylacetate, and Me p-methoxyphenylacetate to
l-decene gives two types of products. In addition to the expected
a-branched esters, dehydrodimer (both meso and dl) esters were also
obtained. The highest yield of a-branched ester was obtained from
I. Higher yields of the dehydrodimer esters were obtained from the
substituted phenyl esters. Attempts to add Me p-nitrophenylacetate to
l-decene were not successful and no evidence for the formation of a
dehydrodimer product was observed.
25169-83-9P 25169-84-0P
RNL: SPN (Synthetic preparation): PREP (Preparation) 25|05-83-97 (5)05-84-07 RE: SPN (Synthetic preparation): PREP (Preparation) (preparation of) 25|05-83-97 (APLUS Butanedioic acid, 2,3-bis(4-methylphenyl)-, dimethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

25169-84-0 CAPLUS Butanedioic acid, 2,3-bis(4-methylphenyl)-, dimethyl ester, (R^*,R^*) - (9CI) (CA INDEX NAME)

Relative stereochemistry

ANSWER 132 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
1967:481889 CAPLUS
67:81889
67:15415a,15418a
67:15415a,15418a
67:15415a,15418a
Reaction of potassium cyanide with p-phenylsulfonylbenzyl bromide
Lotspeich, F. J.
West Vieginia Univ. Med. Center, Morgantown, WV, USA
Journal of Organic Chemistry (1967), 32(4), 1274-7
CODEN: JOCEAN; ISSN: 0022-3263
JOURNAL
English
p-Phenylsulfonylbenzyl bromide (I) is treated with KCN to give
a,-bis (p-phenylsulfonylbenzyl)-p-phenylsulfonylbenzyl
cyanide. I treated with NaI in Me2CO gives p-Ph502C6H4CH2I. Also prepared,
from p-Ph502C6H4COC1 and CH2N2, is p-Ph502C6H4CH2I2. Also prepared,
from p-Ph502C6H4COC1 and CH2N2, is p-Ph502C6H4COCH2N2 which is treated
with Ag2O to give p-Ph502C6H4COC2H.
7705-67-17
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of)
7705-67-1 CAPLUS
Propionic acid, 2,3-bis[p-(phenylsulfonyl)phenyl]-, methyl ester (8CI)
(CA INDEX NAME)

L4 AN DN OREF TI 6b:13265a,13266a
Infrared and ultraviolet spectra of organomercury compounds. II.
Ultraviolet spectra of ethyl a-bromomercuriarylacetates
Artamkina, G. A.; Beletskaya, I. P.; Pentin, Yu. A.; Reutov, O. A.
State Univ., Moscow, USSR
Zhurnal Organicheskoi Khimii (1966), 2(8), 1329-34
CODEN: 20KAE; ISSN: 0514-7492
Journal
Page 10 Journal Russian of CA 63, 13024f. Uv spectra were reported for XC6H4CH(HgBr)CO2Et where X e H, Me, I, NO2, Et, iso-Pr, tert-Bu, F, Cl, and Br in the para position, Me or Br in the ortho position, and Br or Me in the meta position. These esters had 2 characteristic bands at 208-217 and 252-260 m. A comparison with XC6H4CH2CO2Et and XC6H4CHBCO2Et was mader the substituents on the CH2 bridge affect the spectra more significantly than do the ring substituents.

15098-17-6 RELUS (spectrum (uv) of) 15098-17-6 CAPLUS (SUB) (SUB) (CA INDEX NAME) Succinic acid, 2,3-di-p-tolyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME) ΙT

ANSWER 133 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1967:70525 CAPLUS 66:70525 66:13263a,13266a

L4 ANSWER 134 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN AN 1966:429366 CAPLUS DN 65:29366 OREF 65:5434e-f II Flavanoids. II. Stereochemistry of isoaurones AU Marathe, K. G.: Byrne, M. J.; Vidwans, R. N. Univ. Poona, India 65:29366

Flavanoids. II. Stereochemistry of isoaurones
Marathe, K. G.: Byrne, M. J.: Vidvans, R. N.
Univ. Poona, India
Tetrahedron (1966), 22(6), 1789-95

CODEN: TETRAB: ISSN: 0040-4020
Journal
English

cf. CA 54, 3402a. Isoaurones (anhydrolactones of 2-hydroxy-abenzylmandelic acids), trimethylanhydrohazeyl lactone and its
5-methyl-4'-methoxy analog are shown to be trans-stilbene derivs. and are
isomerized to the cis compds. by pyridine. The stereochemistry has been
established by a stereoselective synthesis of the derived
cis-stilbene-a-carboxylic acid and confirmed by uv and N.M.R.
studies. A mechanism for isomerization has been suggested.
6581-70-0 6600-69-7

(Derived from data in the 7th Collective Formula Index (1962-1966))
6581-70-0 CAPLUS

Mandelic acid, 2-methoxy-a-(p-methoxybenzyl)-5-methyl-, ethyl ester
(7CI, 8CI) (CA INDEX NAME)

6600-69-7 CAPLUS Mandelic acid, 2-ethoxy-α-(ρ-methoxybenzyl)-5-methyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

6581-74-4P, Lactic acid, 3-(p-methoxyphenyl)-2-(6-methoxy-m-tolyl), methyl ester
RL: PREP (Preparation)
(preparation of)
6581-74-4 CAPLUS
Mandelic acid, 2-methoxy-α-(p-methoxybenzyl)-5-methyl-, methyl ester
(8CI) (CA INDEX NAME)

L4 ANSWER 135 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1966:429365 CAPLUS
DN 65:29365
OREF 65:5434a-e
TI Heraclenin from Hippomarathrum -AU Kerimov, S. Sh.
CS V. L. Komarov BobSO Zhurnal P--

bos: 3434-e Heraclenin from Hippomarathrum microcarpum Kerimov, S. Sh. V. L. Komarov Botan. Inst., Leningrad Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) (1966), 39(3), 660-6 CODEN: ZPXHAB: ISSN: 0044-4618

LA Russian

(I For diagram(s), see printed CA Issue.

AB Heraclenin (1), m. 107-8°, [e]22D 25.5° (c 2.51,
pyridine), was extracted from H. microcarpum (II). II was extracted with

CHCl3 to

give 200 g. extract, which was dissolved in a min. quantity of CHCl3 and
chromatographed on a column containing neutral Al2O3. The substances were
eluted from the column with petroleum ether, b. 40-60°, with a
petroleum ether-CHCl3 (4: 1) mixture, or with CHCl3 and with HeOH. Elution

with a petroleum ether-CHCl3 mixture gave 2 substances. After evaporation

which a periodous control of the eluate, the residue was dissolved in 4:1 EtOH-CHCl3 to give hydroxypeicedanine. The mother liquor gave crystals which were recrystd. from 4:1 alc.-petroleum ether to give I, m. 107-8*, [a]22D 25.5* (c 2.51, pyridine), Rf 0.31. I (2 g.) added to a hot solution of 0.3 g. (CO2H)2 in 20 ml. H2O, the mixture refluxed 45 min., cooled,

of 0.3 g. (CO2H)2 in ZO ml. hzv, the missive collection of 0.3 g. (CO2H)2 in ZO ml. hzv, the missive collection chromatographed on an inactive Al2O3 column, and eluted with CHCl3 and ETCH, and the EtCH eluate evaporated to give I hydrate, m. 114-15°, v. 3400 cm.-1, Amax 220, 250, 362, 300 ms. I (0.5 g.) was added to 225 ml. 100 HESO4, and the mixture boiled 15 min., filtered hot, and cooled to give isoheraclenin, m. 132.5-4.5° (EtCH), Amaximum 220, 250, 262, 300 ms., Rf 0.25. I (0.2 g.) was dissolved in 10 ml. AcCH, 5 drops concentrated H2SO4 added, the mixture heated on a water bath 1 hr..

left overnight, and diluted with ice water, a yellow product separated, chromatographed on inactive Al203, and eluted with 20:1 Me2COAcOH, the eluate evaporated and the residue crystallized to give xanthotoxol (III), m. 240-1' (Etch), Amaximim 224, 250, 268, 308 pm, Rf 0.73. III (0.2 g.) was dissolved in 6 ml. MeOH, 0.1NKOH added to weak alkaline rice.

(Derived from data in the 7th Collective Formula Index (1962-1966)) 6581-70-0 CAPLUS

Mandelic acid, 2-methoxy-a-(p-methoxybenzyl)-5-methyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

ANSWER 134 OF 146 CAPLUS COPYRIGHT 2007 ACS On STN

ANSWER 135 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

6600-69-7 CAPLUS Mandelic acid, 2-ethoxy-α-(p-methoxybenzyl)-5-methyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

Ł

Synthesis of some organomercury salts of the type XCGH4CH(HgBr)CO2Et Beletskaya, I. P.; Artamkina, G. A.; Shevlyagina, E. A.; Reutov, O. A. Zhurnal Obshchei Khimii (1964), 34(1), 321-4
CODEN: ZOXHA4: ISSN: 0044-460X

Journal

Unavailable cf. CA 57, 16645e. o-BrC6H4CH2CN refluxed in EtOH-concentrated H2SO4 5 h.

Onavalable

of. CA 57, 16645e. o-BrC6H4CH2CN refluxed in EtOH-concentrated H2SO4 5 h.

77% o-BrC6H4CH2CO2Et (I), b7 128°, m. 34.5°. Similarly was prepared the m-isomer, 75%, b2 120-1°, n20D 1.5348, d20 1.3810. p-EtC6H4CH2CO2Et, b4 110°, 1.4970. 1.013, was prepared in 82% yield from the acid and EtOH. I in CC14 was brominated under an incandescent lamp and gave XC6H4CHECC2Et [II] (X = 0-Br), 50%, b1 107°, 1.5781, 1.7266. Similarly was prepared the m-isomer, 60%, b1 104°, 1.5781, 1.7266. Similarly was prepared the m-isomer, 60%, b1 104°, 1.5781, 1.7010, and II (X = 9-02N), 55%, b4 165°, 1.5580, -. Et p-ethylmandelate and PBrJ in CHC13 at first with cooling, then 0.5 h. on a steam bath, gave 73% p-EtC6H4CH(HBC02Et, b4 125°, 1.5350, 1.3227. Similarly were prepared 60% p-iso-Pr analog, b6 142°, 1.5260, 1.2800, and p-methoxy analog, 65%, b3 150°, 1.5500, 1.4050. Shaking II with Hg gave 51% p-MeC6H4CH(HgBr)CO2Et (III), m. 70°, 50% o-bromo analog, m. 91°, 40% m-bromo analog, m. 69°, 70% p-Et analog, m. 95°. In case the product precipitated as an oil, indicating the formation of R2Hg. the mixture was treated with HgBr2 to effect conversion to RHgBr. If the preparation of III was run at 50-60°, the product was 60% (p-MeC6H4CHCO2Et)Z, m. 151°. Similarly was obtained the p-ethylphenyl analog, 15%, m. 125°. The reaction of the p-anisyl member with Hg gave only a tar that was free of Hg. A previously reported substance (loc cit.), m. 145°, was shown to be BrigGT2C6H4CH2CO2Et, rather than III. 15098-17-6F, Succinic acid, 2,3-di-p-tolyl-, diethyl ester RL: PREP (Preparation of) 15098-17-6 CAPLUS Succinic acid, 2,3-di-p-tolyl-, diethyl ester RL: PREP (Preparation of) 15098-17-6 CAPLUS Succinic acid, 2,3-di-p-tolyl-, diethyl ester RL: PREP (Preparation) (preparation of)

95699-75-5 CAPLUS Succinic acid, 2,3-bis(p-ethylphenyl)-, diethyl ester (7CI) (CA INDEX NAME)

ANSWER 137 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1963:66251 CAPLUS

58:66251

DN 58:66251

OREF 58:11265g-h, 11266a-h, 11267a-f

TI Reaction of diazomethane with double bonds. I. Direct methylation of trisubstituted tehylenes

AU Alguero, M.: Bosch, J.: Castaner, J.: Castella, J.: Castella, J.: Mestres, R.: Pascual, J.: Serratosa, F.

CS Univ. Barcelona, Spain

ODEM: TETRAB: ISSN: 0040-4020

DT Journal NAB:

Journal Unavailable

Unavailable

For diagram(s), see printed CA Issue.

cf. CA 57, 12455d. Treatment of "phenzylidene-acarboxybutenolide (I, R = COZH, (R' = H) (4.0 g.) in 15 ml. Et20 at
20° with 2.2-2.4 moles CHZN2 in Et20 and the product recrystd. from

Et20 (or EtOAc) gave 3.8 g. y-benzylidene-a-carbomethoxymethylbutenolide (II, R = COZHe, R' = H) (III), m. 156-8°, µ,

1786, 1726 cm.-1 (CC14), A 202, 227 mm (s. 14,500, 7180),
also produced (0.3 g.) by trestment of I (R = COZHe, R' = H) (0.3 g.) in

Et20 with 1.2-1.4 moles CHZN2 in Et20. Similarly were prepared II (R, R'
and m.p. given): CN, H, 187-90': COZHe, Me, m. 154-7':

COZMe, Cl, 175.0-7.5', COZMe, NO2, 166-72' (decomposition). I (R

= R' = H) (0.2 g.) treated with excess CHZN2 in Et20 gave unchanged

starting material. III (7.23 g.) heated 10 hrs. (N atmospheric) in 200 ml.

dioxane and 80 ml. concentrated HCl and the washed (alc., H20) precipitate

ystd.

refluxed 13 hrs. in 12 ml. MeOH and treated with EtoAc, the filtered solution washed with 2N aqueous K2CO3 and H2O, percolated through an Al2O3 column and the eluate evaporated gave III, also obtained by methylation of IV with ethereal CH2N2. The acids II (R = CO2H, R' = Me, Cl), m. 202-10' (decomposition), A 204, 233, 351 mu (e 16,700, 10,130, 37,900), and m. 208-18' (decomposition), A 202, 234, 342-3 mu (e 12,330, 12,500, 32,700), were similarly prepared IV (2.0 g.) heated in vacuo at 250' and the product distilled at 210'/18 ma. gave 0.8 g. solid, recrystd. from Et2O to give II (R = R' = H) (V), m. 101-3', v. 1786, 1387 cm.-1 (CC14), A 226, 240, 324 mu (e 9150, 7960, 20.490). V (1.0 g.) in 20 ml. 401 HI and 20 ml. AcOH heated 6 hrs. at 160' in a sealed tube and the cooled mixture diluted with H2O, treated with a few drops of aqueous NaESO3 and extracted repeatedly with Et2O, the Et2O shaken with aqueous NaESO3 and the alkaline solution acidsfied with 2N HCI, the acid solution extracted with Et2O and the

acidified with 2N HCl, the acid solution extracted with Et2O and the

acidities with an most, see _____
residue on _____
evaporation recrystd. from petr. ether gave 0.96 g. PhCH2COCHMeCH2CO2H

evaporation tecryson. 11-3' (decomposition). VI Me ester (1.3 g.) and 0.28 g. NaH refluxed 6 hrs. in 20 ml. Et20 and the mixture diluted with 40 ml. Et20, acidified, and the H2O-washed solution evaporated gave

0.6 g.
4-methyl-2-phenyl-cyclopentane-1,3-dione, n. 181-3*.
PhCHZCOCHMCOZET (10.0 g.) in 35 ml. CGH6 treated with NaOEt (from 1.15 g.
Na in 15 ml. alc.) and the CGH6 distilled, the mixture refluxed 9 hrs. with

g. BrCH2CO-2Et in 10 ml. C6H6 and acidified with 2N H2SO4, the C6H6 layer washed with 0.5M aqueous NaHCO3 and H2O and distilled in a high vacuum gave

ANSWER 136 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

AMSVER 137 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
g. oil, b0.1 131-2* n220 1.4960. This oily
phchicocome (CO22t1cH2CO2Et (8.18 g.)shaken 24 hrs. with 8.18 ml. 101 KOH in
diowane, the mixt. washed with Et20 and acidified with 2N HCl, extd. with
Et20 and the residue on evapm. recrystd. from 1:3 Et20-petr. ether gave
VI. VI (0.44 g.) and 2.9 g. KOH in 2.5 ml. 801 N2H4.120 and 5 ml.
(MOCHZCH2)20 refluxed 1 hr. and the mixt. slowly distd. to 175*
inner temp., the residual mixt. refluxed 7 hrs. and dild. with H2O, washed
with Et20 and the aq. solm. acidified with 6NHCl, extd. with Et20 and the
H2O-washed and dried ext. evapd., the residue (0.34 g.) chromatographed in
CGH6 over silica gel and eluted with 20: 1 CGH6Et2O gave 0.34 g. oily
phchickCH2CH2CH6CH2. b0.6 210*; anilide m. 109-111*
p-toluide m. 107-8*. EtHgBc (from 2.43 g. Mg) in 80 ml. Et20
stirred (M atm.) with dropwise addn. of 11.2 g. Phc.tplbond.CH in 20 ml.
dry CGH6 and the mixt. refluxed 2 hrs., treated dropwise at 20*
vith 12.7 g. N-acceptylipperidine (VIa) in 50 ml. dry CGH6 and stirred 17
hrs., extd. 3 times with 100 ml. Et20 snd the exto-vashed shien 24*
hrs., extd. 3 times with 100 ml. Et20 snd the exto-vashed shien 24*
hrs., extd. 3 times with 100 ml. Et20 snd the exto-vashed shien 24*
hrs., extd. 3 times with 100 ml. Et20 snd the exto-vashed shien 24*
hrs., extd. 3 times with 100 ml. Et20 snd the exto-vashed shien 24*
hrs., extd. 3 times with 100 ml. Et20 snd the exto-vashed shien 24*
hrs., extd. 3 times with 100 ml. Et20 snd the exto-vashed shien 24*
hrs., extd. 3 times 24*
hrs., extd. 3 times with 100 ml. Et20 snd the exto-vashed shien 24*
hrs., extd. 3 times 24*
hrs., extd. 3 times with 100 ml. Et20 snd the exto-vashed shien 24*
hrs., extd. 3 times 2

ANSVER 137 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (C2C14), 0.36 g. V, and 0.10 g. mixt. An attempted synthesis of 1-methyl-3-phenylpropargylidenemalonic acid (for further cyclization to a-carboxy-p-methylbutenolide) by condensation of VII and RCC(C221) 2 gave a neg. result. VII (0.38 g.), 0.67 g. NCCH2CO2H, and 2 ml. AcOH neated (N atm.) 82 hrs. at 100° and didle with 3 ml. HZO and 3 ml. petr. ether, filtered, and the washed residue recrystd. from CRH6 gave 0.15 g. II (R - Cx, R = H), hydrolyzed (0.10 g.) by heating 3 hrs. at 100° in 2.5 ml. AcOH and 3 ml. 60H HZO4 to IV. The p-methylbutenolide structure of the compds. I and II was also established by a study of their hydrogenated derivs. (VIII). IV (200 mg.) in 33 ml. abs. alc. and 2 ml. HZO contg. 75 mg. XOH hydrogenated at 14'752 m. with 33 mg. PtO2 and adsorption of 2.08 moles H, the mixt. treated with 0.27 ml. 2N HCl and the filtered soln: evapd. in vacuo, the residue taken up in 30 ml. 120, acidified with ZN HCl, extd. with 1:10 CHC13-HZO, and the oily product tubbed with BtZO gave 90 mg. VIII (R = COZH) (IX), m. 123-77, v. 1783, 1721 cm.-1 (CH-C13). The EtZO soln. extd. with aq. NaHCO3 and the alk. ext. acidified, extd. with EtZO, and the sirupy product chromatographed over silica gel yielded 40H stereoisomeric mixt. of acids. III (2.0 g.) in 75 ml. alc. hydrogenated over 0.1 g. PtO2 and the filtered soln. evapd. gave a colorless, fluid resin VIII (R = COZH), b0.01 140°, refluxed (2.0 g.) with 2.0 g. VIII (R = H) (X), b0.75 130°, v 1779 cm.-1 V (1.0 g.) in 50 ml. alc. hydrogenated over 0.0 ml. arc and the filtered soln. evapd. gave a colorless oil, b0.75 130°, possibly isomeric with X or a mixt. X (2.0 g.) with 120 ml. alc. the Y in vacque and the residue distd. gave 0.8 g. VIII (R = H) (X), b0.75 130°, v 1779 cm.-1 V (1.0 g.) in 50 ml. alc. hydrogenated over 60 mg. Pro2 and the filtered onle word, gave a colorless oil, b0.75 130°, v 1779 cm.-1 V (1.0 g.) in 50 ml. alc. hydrogenated verve 60 mg. Pro2 and the filtered onle veryet of the produ

ANSWER 137 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 98333-22-3 CAPLUS Succinic acid, 2-m-toly1-3-p-toly1-, diethyl ester (7CI) (CA INDEX NAME)

98333-28-9 CAPLUS

Succinic ac INDEX NAME) cinic acid, 2-(p-methoxyphenyl)-3-p-tolyl-, diethyl ester (7CI) (CA

ANSWER 137 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) 15098-17-6 CAPLUS SUccinic acid, 2,3-di-p-tolyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME)

97116-28-4 CAPLUS Succinic acid, 2,3-di-o-tolyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)

97116-29-5 CAPLUS Succinic acid, 2-o-tolyl-3-p-tolyl-, diethyl ester (7CI) (CA INDEX NAME)

98333-21-2 CAPLUS Succinic acid, 2,3-di-m-tolyl-, diethyl ester (7CI) (CA INDEX NAME)

ANSWER 138 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1962:483341 CAPLUS 57:83341

DN 57:83341
OREF 57:16645e-h
TI Synthesis of some organomercury salts of type XCGH4CH(HgBr)CO2C2H5.II
AU Beletskaya, I. F.: Reutov, O. A.; Artamkina, G. A.
S Zhuranal Obshchet Xhimii (1962), 32, 241-4
CODEN: ZOKHA4; ISSN: 0044-460X
DJ Journal
LA Unavailable

Unavailable
cf. CA 55, 21014b. Adding 18 ml. Br to 55 g. p-FC6H4CH2CO2H and 2.8 g.
red P in refluxing CHCl3, refluxing until HBr evolution ceased, and adding
23 ml. Br with heating gave after heating with 30 ml. EtOH followed by

red P in refluxing CHCl3, refluxing until HBr evolution ceased, and addi 23 ml. Br with heating gave after heating with 30 ml. EtcH followed by 1003

23 ml. Br with heating gave after heating with 30 ml. EtcH followed by 1004

29°, and 22% p-FCGH4CHBrCOZEt, b0 120-2°, n200 1.5190, d20

1.4623. Similarly were prepared: p-BrCGH4CHBrCOZEt, 55%, b3 130-2°, 1.5579, 1.6600; p-ICGH4CHBrCOZEt, 10%, m. 52°; p-ICGH4CH2COZET, 25%, n. 29°. The residue from the last substances treated with Et20 gave Et02CCH(CGH41-p)CBrCGH4CH-p)COZET (provisional structure), m. 130°, and less soluble in Et20, (p-ICGH4CHCOZET) 2 m. 170-1°.

Also were prepared: 55% o-MeCGH4CHBrCOZET, b7 132-4°, 1.5397, 1.3721; 53% m-isomer, b4 130-2°, 1.5348, 1.3536; 76% p-Me3CCGH4CHBrCOZET, b2 140-2°, 1.5300, 1.2660; 5% p-Me3CCGH4CHZCOZET, b3 100-10°, 1.5030, 0.9800. Addition of Br to I in CCI4 under incandescent lamp illumination gave 85% p-FCGH4CHBrCOZET (11), b3 105-6°, 1.5190, -. Similarly were prepared: p-Cl analog, 75%, b5 138-40°, 1.5503, -; p-I analog, 76%, b3 130-3°, 1.5580, -; p-I analog, 44%, m. 52°. II shaken 4 hrs. with Hg gave 24% p-FCGH4CH(HgBF)COZET, 75%, m. 94°; p-Me3CGH4CH(HgBF)COZET, 75%, m. 94°; p-Me3CGH4CHHgBF)COZET, m. 110°; m-MeCGH4CH(HgBF)COZET, 75%, m. 94°; p-Me3CGH4CHHgBF)COZET, m. 110°; m-MeCGH4CHHgBF)COZET, 75%, m. 94°; p-Me3CGH4CHHgBF)COZET, p. 90°; m. 90°; m. 90°; m. 90°; m. 90°; m. 9

94550-49-9 CAPLUS Succinic acid, 2-bromo-2,3-bis(p-iodophenyl)-, diethyl ester (7CI) (CA INDEX NAME)

ANSWER 138 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

L4 ANSWER 139 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

114791-94-5 CAPLUS

114791-94-5 CAZLOS 4H-1-Benzopyran-6-acetic acid, a,5,7-trihydroxy-a-p-hydroxybenzyl-2-(p-methoxyphenyl)-4-oxo-, ethyl ester (6CI) (CA INDEX NAME)

115099-51-9 CAPLUS
4H-1-Benzopyran-6-acetic acid, a,5-dihydroxy-7-methoxy-a-p-methoxybenzyl-2-(p-methoxyphenyl)-4-oxo-, ethyl ester (6CI) (CA INDEX NAME)

L4 ANSYER 139 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1961:17917 CAPLUS
DN 55:17917
OREF 55:3579a-f
T1 The structure of ginkgetin. V. Flavone carboxylic acid
AU Kogure, Akira
CS Osaka City Univ.
SO Nippon Kagaku Zasshi (1959), 80, 1462-6
CODEN: NPRZAZ; ISSN: 0369-5387
DT Journal Nippon Kagaku Zasshi (1959), 80, 1462-6
CODEN: NPKZAZ: ISSN: 0369-5387
Journal
Unavailable
A flavonecarboxylic acid. C25H2009 (I), was obtained from ginkgetin (Ia)
by treating with KOH-H2O, which gave the Me ether Me ester (II) with CH2N2
(cf. preceding abstract). II showed pos. FeCi3 reaction, & 2.71,
3.21, 5.8, 6.00 M, suggesting the existence of still more hydroxy
groups. II heated with Ac2O and AcONa gave the wo accetates, C30H2608, m.
139-141', and C32H30011, m. 196-8'. II gave the carboxylic
acid Me ether (III), C27H2409, pale yellow, insol. in NaHCO3 solution III
gave C27H2208, m. 216-18', yellow, supposedly a dehydrated III, by
boiling with MeOH-HCL. I with ale. H2SO4 gave the Me ester. C27H2409,
yellow, m. 188-190', reconverted to I by hydrolysis and converted
to the Me ether, m. 220-2', by CH2N2, then further to III by
hydrolysis. I gave the acetate. C3H280013, m. 222-4', by
acetylation and the Me ether Me ester (IV), C30H3009, m. 221-2',
different from II, with MeZSO4. IV had no carbonyl group other than one
in the y-pyrone ring, since IV did not form the oxime under mild
conditions. IV was hydrolyzed to a flavonecarboxylic acid Me ether (V),
C29H2809, m. 298', converted to the Et ester, C3H3209, m.
208-210', by treating with alc. HCL. In an attempt to
decarboxylate by boiling with quinoline and Cu, IV was recovered unchanged
or decomposed, indicating that the carboxy group in IV was not attached to
the double bond. Heating V at 305' 7-8 min. gave the flavone
lactone (VI), C27H2209, m. 215-16', by demethylation and
dehydration, green with FeCl3. VI yielded the acetate, C29H2409, m.
185-7'. Hydrolysis of VI with 5% ale. KOH gave a flavonecarboxylic
acid (VII), C27H2209, m. 298-300'. IV was prepared by methylation in 46
dehydration, green with FeCl3. VI yielded the acetate, C9H2409, m.
185-7'. Hydrolysis of VI with 5% ale. KOH gave a flavonecarboxylic
acid (VII), C27H2209, m. 298-300'. IV was prepared by methylation in 46
dehydration, green with FeCl3. VI yielded the acetate, C9H2409, m.
185-7'. Hydrol t

IV). Demethyl derivative of Ia, m. above 320°, gave demethyl derivative of I, which yielded IV with MeSO4. The structure of Ia was supposed to be a flavone nuclearly fused with a hydroflavonol.

114696-94-5 114791-94-5 115099-951-9

(Derived from data in the 6th Collective Formula Index (1957-1961))

114696-94-5 CAPLUS

4H-1-Benzopyran-6-acetic acid, a,5-dihydroxy-7-methoxy-a-p-methoxybenzyl-2-(p-methoxyphenyl)-4-oxo-, methyl ester (6CI) (CA INDEX NAME)

ANSWER 140 OF 146 CAPLUS COPYRIGHT 2007 ACS ON STN 1961:17916 CAPLUS 55:17916

DN 55:17916
OREF S5:3578i,3579a-b
TI The structure of ginkgetin. IV. Alkali cleavage of ginkgetin
AU Kogure, Akira
C Osaka City Univ.
SO Nippon Kagaku Zasshi (1959), 80, 1355-8
CODEN: NPKZAZ; ISSN: 0369-5387

CODEN: NPKZAZ; ISSN: 0369-5387

Journal

Unavailable

Ginkgetin (1) boiled 40 min. in 30% aqueous KOH solution gave
p-methoxyacetophenone (II), anisic acid (III), flavonecarboxylic acid

(IV), C25H2909, m. 308-10°, and oxoflavone (V), m. 269°

(decomposition). I boiled in 40% aqueous KOH solution many hrs. gave

ic acid, II,

III, and phloroglucinol. IV, C25H2009, brown with FeCl3, red with HCl-Mg,

was converted to the Me ether Me ester, C28H2609, m. 214-15°, brown

with FeCl3. V gave the oxime, m. 275-6°, and the semicarbazone, m.

228-30°. V gave the mono-Me ether, C27H2207, m. 220-2°,

green with FeCl3, converted to the acetate, C29H2409, m. 224-6.5°.

IV and V exhibited ultraviolet absorption essentially identical with that

of I.

of I.
114696-94-5 114791-94-5 115099-51-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
114696-94-5 CAPLUS
4H-1-Bencopycan-6-acetic acid, a,5-dihydroxy-7-methoxy-a-p-methoxybenzyl-2-(p-methoxyphenyl)-4-oxo-, methyl ester (6CI) (CA INDEX

114791-94-5 CAPLUS
4H-1-Benzopyran-6-acetic acid, e,5,7-trihydroxy-e-p-hydroxybenzy1-2-(p-methoxyphenyl)-4-oxo-, ethyl ester (6CI) (CA INDEX NAME)

115099-51-9 CAPLUS 4H-1-Benzopyran-6-acetic acid, α,5-dihydroxy-7-methoxy-α-p-methoxybenzyl-2-(p-methoxyphenyl)-4-oxo-, ethyl ester (6CI) (CA INDEX NAME)

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CAS ONLINE PRINTOUT

L4 ANSWER 140 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 141 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) dihydroxyphenyl)butyric acid (XIII), 220-1", β-(2-methoxy-5-methylphenyl)-β-(2,4-dimethoxyphenyl)butyric acid (XIV) (8 g. from 15 g. of XIII), 116", 165", - (b10 240"); 10 g. IV, 10 g. resorcinol, 10 g. hydroxybutyrolactione of β-(2-methoxy-4-methylphenyl)-β-(2,4-dimethoxyphenyl)butyric acid (XV), 190" (methoxy deriv., m. 183"), β-(2-methoxy-4-methylphenyl)-β(2,4-dimethoxyphenyl)butyric acid (XVI), 116-17", 132", (b15 160"). Both, β,β-bis (p-methoxyphenyl)butyric acids, as well as β-(p-methoxyphenyl)butyric acids, as well as β-(p-methoxyphenyl)butyric acids, on distn. with lime at 3 mm. lost a mol. of AcOH and gave α,α-bis(substituted-phenyl)ethylenes, but β,β-bis(o-methoxyphenyl)butyric acids, on distn. with lime at 3 mm. lost a mol. of AcOH and gave α,α-bis(substituted-phenyl)ethylenes, but β,β-bis(o-methoxyphenyl)butyric acids, the following were the results of distn. with lime of the various butyric acid derivs, preput (butyric acid deriv., product obtained, m.p. given): III, α,α-bis(4-methoxy-3-methylphenyl)-α'-(4-methoxy-3-methylphenyl)-α'-(4-methoxy-4-methylphenyl)-α'-(4-methoxy-3-methylphenyl)-α'-(4-methoxy-3-4-methylphenyl)-α'-(4-methoxy-3-4-methylphenyl)-α'-(4-methoxy-3-4-methylphenyl)-α'-(4-methoxy-3-methylphenyl)-α'-(4-methoxy

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L4 ANSWER 141 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1960:56237 CAPLUS
DN 54:56237 CAPLUS
DN 54:56237
OREF 54:10941d-1,10942a-d
TI Ellination of acetic acid during decarboxylation of organic acids. II.
Formation of a, a-diarylethylenes from β,β'diarylbutyric acids
AU Gogte, G. R.; Kasarakar, D. Y.
S Inst. Sci., Bombay
SJ Journal of the University of Bombay, Science: Physical Sciences,
Mathematics, Biological Sciences and Medicine (1958), 27(No. 3), 41-54
CODEN: JUBSAS; ISSN: 0368-4664
JOurnal
LA Unavailable
AC G. C.A. 54, 8717b. The preparation of variously substituted
β,β-diarylbutyric acids and their behavior on distillation with lime
was described. A mixture of 32 cc. AccH2COZET (1) and 31 cc. o-cresol Me
ether (II) cooled to 0-5°, 200 cc. 70% H2SO4 added gradually with
shaking, the mixture left 8 hrs. at room temperature, poured on crushed ice

the semisolid lump hydrolyzed by refluxing 2 hrs. with 160 cc. aqueous 30%
NaOH and 100 cc. MeOH gave 16 g. β,β-bis(4-methoxy-3methylphenyl)butyric acid (III), m. 127', smilide m. 143';
Et ester, m. 65°. 2-Methoxy-4-methyl-β-methylcinnamic acid
(IV), m. 139' (EtcM), obtained by an alkaline hydrolysis of
4,7-dimethylcoumarin, similarly condensed with II and anisole, resp., gave
β-(2-methoxy-4-methylphenyl)-β-(4-methoxy-3-methylphenyl)butyric
acid (V), m. 120-1' (anilide m. 139'; Et ester m.
62'), and β-(2-methoxy-4-methylphenyl)-β-(4methoxyphenyl)butyric acid (VI), m. 162' [anilide m. 136';
Et ester m. 60' (MeOH)), Similarly, 20 g. 2-methoxy-5-methylphenyl)β-methylcinnamic acid (VII) (Auvers, C.A. 11, 2325) condensed with 24
cc. anisole gave 19 g, β-(2-methoxy-5-methylphenyl)-β-(4methoxyphenyl)butyric acid (VII), m. 162' [anilide m. 153',
Et ester bl 7270'. However, 10 g, VII condensed likevise with 6
cc. p-cresol gave 5 g, butyrolactone of β-(2-methoxy-5methylphenyl)butyric acid (VII), m. 163', anilide m. 153',
Et ester bl 7270'. However, 10 g, VII condensed likevise with 6
cc. p-cresol gave 5 g, butyrolactone of β-(2-methoxy-5methylphenyl)-β-(2-hy

ith 2N cc. concentrated HC1, diluted with 100 cc. H2O, adjusted to pH 5.0 ith 2N NaOH, and filtered, and the residue repptd. from AcOH-HC1 at pH 5.0, and recrystd. from aqueous CSHSN yielded the corresponding 4,3,5-ArO(02N)2CGHZCHZCH(NH2)CO2H (Ar. 4 yield, and m.p. given): o-MeCGH4, 23, 192-3* (hygroscopic): 2.5-MeZCGH3, 13, 211-14*; o-iso-PtCGH4, 8, 187-90*; 2,5-iso-PtMeCGH2, 60, 196-9*. The appropriate II (0.02 mole) in 300 cc. AcOH hydrogenated 45 min. at 35 lb. initial pressure over 2.0 g. 10% Pd-C, treated with 15 cc. concentrated 2504.

H2SO4,
filtered, added with stirring during 2 hrs. to 5.6 g. NaNO2 in 120 cc.
concentrated H2SO4 and 40 cc. AcOH at -5°, stirred 2 hrs. at -5°,
treated with stirring at 25° with 17 g. iddine and 12 g. NaI in 300
cc. H2O underlayered by 300 cc. CHC13, the aqueous phase extracted after 2

with CHCl3, and the combined CHCl3 solns, worked up yielded the corresponding 3,5,4-12(ArO)CGH2CH2CH(NHAC)COZEt (III) (Ar, 1 yield, and m.p. given): o-MeCGH3, 61, 111-12' (aqueous EtOH): 2,4-Me2CGH3, 55, 139-40' (aqueous EtOH): 2,5-Me2CGH3, 33, 147-8' (aqueous Me2CO): 4,2,3-CLMe2CGH2, 57, 175-6' (aqueous EtOH): 4,2,5-CLMe2CGH2, 61, 153-4' (aqueous EtOH): o-iso-PrCGH4, 57, 142-3' (aqueous Me2CO): 2,5-iso-PrCMeCGH3, 55, 178-9' (aqueous EtOH): 2,4-Me(MeO)CGH3, 57, 150-1' (aqueous EtOH): 2,5-Me2(MeO)CGH2, 52, 163-40' (aqueous EtOH): 2,5-Me2(MeO)CGH2, 52, 163-40' (aqueous EtOH): 2,5-Me2(MeO)CGH2, 52, 163-40' (aqueous EtOH): The appropriate III (4.1 mmoles), 25 cc. glacial AcOH, and 25 cc. concentrated HCl refluxed

hrs., cooled, adjusted to pH 5.0 with 2N NaOH, and filtered, the residue dissolved in hot aqueous pyridine and repptd. with 2N HCl at pH 5, the reppth.

reppin.
repeated, and the crude product again repptd. from N NaOH in 50 or 75%

1

ANSWER 142 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
ETOH at pH 5.0 with 2N HCl in the presence of a few drops 2N NaOAc yielded
the corresponding 3,5,4-12 (ArO)CGHZCH2CH(NHZ)COZH (IV) (Ar. & yield, and
ap., with decompn. given): o-MeCGH4, 87, 234-7°; 2,4-Me2CGH3, 88,
190-2°; 2,5-Me2CGH3, 56, 196-7°; 4,2,3-CLMe2CGH2 (crystg.
with lacole H2O), 71, 213-14°, 4,2,5-CLMe2CGH2 (crystg.
with lacole H2O), 71, 213-14°, 4,2,5-CLMe2CGH2 (crystg.
H2O), 71, 205-7°, o-iso-PrCGH4, 50, 202-5°,
2,5-iso-PrMeCGH3, 78, 183-5°. The appropriate III (9.5 mmoles), 40
cc. glacial AcOH, and 30 cc. 58% HI refluxed 8 hrs., concd. to near
dryness at 50°/5 mm, dissolved in a suspension of Na2S2O5 in hot
EtOH, treated with addnl. Na2S2O5 until decolorized, adjusted with 2N
NaOAc to pH 5.0, and centrifuged, and the ppt. repptd. from NaOH in 50%
EtOH at pH 5.0 with 2N HCl gave the corresponding IV (Ar. & yield, and
mp. with decompn. given): 2,4-Me(H0)CGH3 (V), 67, 227-9°,
2,5,4-Ne2(H0)CGH2 (VI), 87, 199-201°, 2,4-iso-Pr(H0)CGH3 (VII), 87,
184-6°; 2,5,4-iso-Pre(H0)CGH2 (VII), 67, 190-1° V (2.0
g.) in 40 cc. 33% aq. EtNH2 treated with 5.1 cc. aq. soln. of 2.55 g.
iodine and 4.0 g. XI during 2 hrs. at room temp., stirred 1 hr., adjusted
to pH 5 with AcOH, and centrifuged, and the ppt. repptd. 3 times from N
NaOH in 50% EtOH at pH 5.0 with 2N HCl contg. a few drops aq. NaOAc,
washed, and centrifuged yielded 2.3 g. 5'-iodo deriv. (IX) of V, light tan
powder, m. 221-4° (decompn.). VII (1.5 g.) in 25 cc. 33% aq. EtNH2
treated during 2 hrs. at room temp. with 5.3 cc. aq. soln. of 2.7 g.
iodine and 4.1 g. XI, stirred 1 hr., and worked up in the usual manner
gave only an incompletely iodinated material: a similar run during 9 hrs.
resulted in less complete iodinated material: a similar run during 9 hrs.
ersulted in less complete iodination than before. VI (0.52 g.) in 20 cc.
33% aq. EtNH2
treated during 1 hr., with 2.0 cc. aq. soln. of 1.0 g. iodic
and 1.3 g. XI, stirred 1 hr., and worked up in the usual manner gave an
incompletely iodinated pr

Optived from data in the 6th Collective Formula Index (1957-1961)) 97116-28-4 CAPLUS Succinic acid, 2,3-di-o-tolyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)

L4 ANSWER 143 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN

ANSWER 143 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1960:11193 CAPLUS 54:11193 54:2241h-i,2242a-c Action of sodamide on α-bromoarylacetates Hoch, Joseph; Choisy, Jean M. Compt. rend. (1959), 248, 3314-16 Journal Unavailable Compt. rend. (1959), 248, 3314-16
Journal
Unavailable
CASRACT 54:11193
The appropriate Grignard reagent reacted with (CO2Et)2 to give the following Et esters (% yield, b15, m.p. given): p-toluoylformate (1), 41, 155°, 132; m-toluoylformate (11), 24, 150°, 112°; o-toluoylformate (111), 26, 145°, 154°; p-methoxybenzoylformate (111), 28, 185, 12°; o-methoxybenzoylformate (111), 38, 185, 12°; o-methoxybenzoylformate (111), 20°, 145°, 154°; p-methoxybenzoylformate (111), 20°, 145°, 151°, p-methoxybenzoylformate (111), 20°, 145°, 151°, p-methoxybenzoylformate (111), 20°, 145°, 151°, p-methoxybenzoylformate (111), 20°, 151°, p-methoxybenzoylformate (111), 20°, 151°, p-methoxybenzoylformate (111), 20°, 151°, p-methoxymandelate (X), 631, m. 46°; Et o-methoxymandelate (X1), 515°, p-methoxymandelate (X), 631, m. 46°; Et o-methoxymandelate (X1), 501, m. 67°. Treatment of 3 moles each of VII-XII with 2 moles PBr3 in varm C6H6 solution converted them to the following: Et p-tolyl-a-bromoacetate (XIII), 511, 513, 513°, 155°, p-methoxyphenyl-a-bromoacetate (XVII), 511, 513°, 513°, Et o-methoxyphenyl-a-bromoacetate (XVII), 681, b2 133°, and Et o-methoxyphenyl-a-bromoacetate (XVII), 681, b2 133°, and Et n-mphthyl-a-bromoacetate (XVII), 681, b2 133°, and Et n-mphthyl-a-bromoacetate (XVIII), 500°, b1 130°, and Et 1-naphthyl-a-bromoacetate (XVIII), 500°, and Et n-naphthyl-a-bromoacetate (XVIII), 500°, and Et n-naphthyl-a 60% material, bl5 240-50°, which was di-Et di-p-tolylmaleate, m. 84°, and di-Et di-p-tolylfumarate, m. 117°. From the non-crystallizable residue, after saponification, there was obtained di-p-tolylfumaleic anhydride and di-p-tolylfumaric acid. XIV gave di-Et di-m-tolylmaleic anhydride, m. 96°, di-m-tolylmaleic anhydride, m. 92-3°, and di-m-tolylfumaric acid, m. 265°. XV gave a fraction, bl5 215-40°, which yielded a small amount di-Et di-o-tolylsuccinate, m. 149°. XVII resetted difficultly and gave noncryst. products which on saponification gave a trace of di-o-methoxyphenylmaleic anhydride, m. 162°. XVIII gave only resinous products. 97116-28-47, Succinic acid, 2,3-di-o-tolyl-, diethyl ester (Preparation of) 97116-28-4 CAPLUS Succinic acid, 2,3-di-o-tolyl-, diethyl ester (6CI. 7CI) (CA INDEX NAM

Succinic acid, 2,3-di-o-tolyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)

ANSWER 144 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN 1959:114554 CAPLUS 53:114554

OREF 53:20554d-e TI Pharmacolog AU Oyaizu, Sus 53:20554d-e Pharmacology of organic acid esters and amides Oyaizu, Susumu Univ. Kyonkyu (1958), 30, 108-19 CODEN: YKKOKA; 155N: 0372-7734

Journal Unavailable Pharmacol.

Unavailable
Pharmacol. action of over 20 derivs. of dimethylaminoethyl diphenylacetate
and diphenylajvoolate was examined for possible relation between chemical
structure and pharmacol. activity. No definite relation was found except
in atropine activity; the activity was generally weakened by substitution
of one of the Ph groups with benzyl, substitution of the base with a
heterocylic system, substitution of the phenyl with Cl or MeO at the para
position, and derivation of the ester to its amide. Atropine activity
increased by quaternization of the base, and substitution of dimethyl in
the base with diethyl.
2-dimethylaminoethyl ester
(pharmacology of)
109095-40-1 (Lactic acid, 2,3-bis(p-chlorophenyl)-,
2-dimethylaminoethyl ester
(pharmacology of)
109095-40-1 CAPLUS
Lactic acid, 2,3-bis(p-chlorophenyl)-, 2-dimethylaminoethyl ester (GCI)
(CA INDEX NAME)

L4 ANSWER 145 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1956:77742 CAPLUS
UN 50:77742 CAPLUS
UN 50:77742 CAPLUS
UN 50:77742 CAPLUS
UN 50:77642

TI Nitrogen containing derivatives of esters of meso-o, a'diphenylsuccinic acid
AU Torf, S. F.: Khromov-Borisov, N. V.
S Zhurnal Obshchei Khimii (1956), 26, 856-64
CODEN: ZOXYA4; ISSN: 0044-460X
U JOURNAL CODEN: ZOWHAY; ISSN: 0044-460X Journal Unavailable
The 3 esters of diphenylsuccinic acids containing N, described below, show curare-like activity. To 23.4 g. PhCH2CN and 48.6 g. HBr-free Eto2CCHBrPh was added in 20 min. 4.9 g. Na in 120 ml. EtoH with cooling; after stirring 45 min. and standing overnight the mixture was filtered and the precipitate washed with EtOH and 200 ml. H2O yielding a residue of 37.69 PhCH(CN)CHPKDCZET (I), m. 139-40* (from EtOH). The basic filtrate was concentrated, washed with H2O, and extracted with Et2O yielding 15.4 g. OND. own product, b1-2 76-102°, and 2.8 g. viscous oil, b1-2 165-78°, which gave 0.5 g. I. To 2.4 g. Na in 65 ml. EtOH was added 19.3 g. molten Ph2CHCM and 15 ml. EtOH, the solution was chilled and treated over 20 min. with 24.3 g. EtO2CCHEPTh and 20 ml. EtOH; after 0.5 hr. the mixture was stirred 1 hr. with cooling and kept overnight; the precipitate was filtered and washed with H2O yielding 66.8% Ph2C(CN)CHPhCO2Et, m. 164-5* (crude), m. 165-6* (from EtOH). Hydrolysis of 75 g. (PhCHCN)2 according to Wawzonek (C.A. 34, 3730.3) followed by separation of the resulting acid and conversion to the Ba salt gave a precipitate of racemic salt, while the filtrate containing the Ba salt of the meso form was heated 70° and acidified with HCl yielding 73.1% meso-{PhCHCO2H}2, m. . 227-9°. Boiling the Ba salt of the racemate with dilute H2S04 and separation of BaS04 gave on cooling 19.7% racemic (PhCHCO2H)2 monohydrate, separation of BaSO4 gave on cooling 19.7% racemic (Fruntucan)2 mononyutate, 183-5°. Refluxing I with 1:1 H2SO4 and AcOH 7 hrs., gave some EtOAC; the residue was refluxed 6 hrs. with more AcOH and diluted yielding 92.3% meso-(PhCHCOZH)2, m. 227-9°, which (37.8 g.) with 59.5 g. PCIS and 40 ml. PCCI3 gave on heating to 100° 75.1% meso-(PhCHCOCI)2, m. 186-8°, which refluxed with EtOH gave the di-Et ester, m. 140-1°; Ne2NCHZCH2OH similarly gave the bis(dimethylaminoethyl) ester (II), m. 93-5° (di-HCl salt, m. 239-40°); similarly was prepared bis(diethylaminoethyl) ester (III), m. 58-60° (di-HCl salt, m. 205-6°). II treated with MeI in Me2CO gave the dimethiodide, m. 251-3°; till gave the dimethiodide, m. 225-6°. To 50 ml. HNO3 (d. 1.52) was added with cooling 10 g. meso-(PhCHCOZH)2 at about 0° in 1 hr. and after stirring 0.5 hr. the mixture was quenched with ice, the separated product dried and boiled 1 with 200 ml. AcOH and filtered hot yielding 8.5 g. solid, m. 227-8°, which was taken up in aqueous MH40H, decolorized and treated with hot AcOH yielding 56.4 h meso-(p-02NCGH4CHCO2H), 2, m. 238-40°; this with EtOH-H2SO4 gave after 27 hrs. refluxing 38.8% di-Et ester, m. 159-61°; the same was obtained in 62.7% yield on nitration of the unsubstituted ester above with HNO3 (d. 1.51) at about 0°.

ANSWER 145 OF 146 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) Reduction of the ester with SnC12 2H20 in EtOH in the presence of Ca gave in 5 hrs. 70.2% meso-(p-H2NC6H4CHCO2E1)2. m. 183-5" (crude): m. 186-7" (from CGH6), without added CaCO3 the reaction tends to give a low melting product. This refluxed with Mel in EtOH in the presence of H20 and CaCO3 5 hrs. gave the dimethiodide, m. 212-14" (from H20). The 3 methiodides described above showed curare-like properties.
860426-35-3P, Succinic acid, 2,3-bis(p-aminophenyl)-, diethyl ester

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19 ANSWERS

L5 STRUCTURE UPLOADED

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SAMPLE SEARCH INITIATED 10:04:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 148 TO ITERATE

100.0% PROCESSED 148 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
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PROJECTED ITERATIONS: 2231 TO 3689

PROJECTED ITERATIONS: 2231 TO 3689
PROJECTED ANSWERS: 119 TO 641

L6 19 SEA SSS SAM L5

=> d scan

L6 19 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzenepropanamide, 4-(aminoiminomethyl)-N-[(1S)-1-cyclohexyl-2-[[[1-(1-iminoethyl)-4-piperidinyl]methyl]amino]-2-oxoethyl]-a-[3-(trifluoromethyl)phenyl]-, (aS)CI COM

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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FILE 'REGISTRY' ENTERED AT 08:08:27 ON 27 DEC 2007

L1 STRUCTURE UPLOADED

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L3 1 S L1 CSS

· L4 1 S L1 CSS FUL

FILE 'REGISTRY' ENTERED AT 08:17:29 ON 27 DEC 2007

L5 1 S L1

L6 5 S L1 FUL

FILE 'CAPLUS' ENTERED AT 08:17:45 ON 27 DEC 2007

=> d l1

L1 HAS NO ANSWERS

L1 STR

G1 H,Ak,OH

Structure attributes must be viewed using STN Express query preparation.

=> s 16

L7 12 L6

=> d bib abs hitstr 1-12

L7 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:757334 CAPLUS

DN 139:276885

TI Preparation of novel heterocyclic analogs of diphenylethylene compounds as antidiabetics

IN Neogi, Partha; Dey, Debendranath; Medicherla, Satyanarayana; Nag, Bishwajit; Lee, Arthur

PA USA

SO U.S. Pat. Appl. Publ., 66 pp., Cont.-in-part of U.S. Ser. No. 843,167. CODEN: USXXCO

DT Patent

LA English

FAN. CNT 12

PATENT NO. KIND DATE APPLICATION NO. DATE

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PΙ
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; Z = II-IV; n, m, q and r = 0-4 ($n+m \le 4$ and $q+r \le 4$); p, s = 0-5 (p+s \le 5); R, R2 = H, alkyl, alkenyl, etc.; R1 = H, alkyl, alkenyl, etc.; A, A1, A2 = H, acylamino, acyloxy, alkanoyl, etc.; B, B1, B2 = H, acylamino, acyloxy, alkanoyl, etc.; or A and B together, or A1 and B1 together, or A2 and B2 together, may be joined to form a methylenedioxy or ethylenedioxy; X, X1 = (un)substituted NH, O, S] which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes, were prepared E.g., a multi-step synthesis of V, starting from 3,5-dimethoxybenzaldehyde and 4-hydroxyphenylacetic acid, was given. The compound V showed strong glucose lowering activity even though it is a weak PPAR- γ agonist (data given). The compds. I are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis. Pharmaceutical composition comprising the compound I was claimed. 380881-43-6P IT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of diphenylethylene compds. containing thiazolidinedione or oxazolidinedione moieties for treating diabetes, inflammatory or immunol. disease in combination with other agents)

RN 380881-43-6 CAPLUS

CN Benzenepropanoic acid, α -(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (CA INDEX NAME)

L7 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:645701 CAPLUS

DN 140:87046

TI Synthesis and structure-Activity relationship studies of cinnamic acid-based novel thiazolidinedione antihyperglycemic agents

AU Neogi, Partha; Lakner, Fredrick J.; Medicherla, Satyanarayana; Cheng, Jin; Dey, Debendranath; Gowri, Maya; Nag, Bishwajit; Sharma, Somesh D.; Pickford, Lesley B.; Gross, Coleman

CS Department of Chemistry, Calyx Therapeutics Inc., Hayward, CA, 94545, USA

SO Bioorganic & Medicinal Chemistry (2003), 11(18), 4059-4067 CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 140:87046

GI

Ι

AB A number of 2,4-thiazolidinedione derivs. of -Ph substituted cinnamic acid were synthesized and studied for their PPAR agonist activity. The E-isomer of cinnamic acid, I, showed moderate PPAR transactivation. The corresponding Z-isomer and double bond reduced derivative were found to be much less potent. Although the E-isomer showed a moderate PPARy transactivation, it demonstrated a strong glucose-lowering effect in a genetic rodent model of diabetes. Results of pharmacokinetic, metabolism and permeability studies are consistent with I being an active prodrug with the hydrolyzed carboxylate as an active metabolite that has similar

glucose lowering and PPARy agonist properties.

IT 380881-43-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cinnamic acid-based thiazolidinedione antihyperglycemic agents)

380881-43-6 CAPLUS RN

CN Benzenepropanoic acid, α -(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (CA INDEX NAME)

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:185699 CAPLUS

DN136:247571

Preparation of novel heterocyclic analogs of diphenylethylene compounds as ΤI inhibitors of cytokines or cyclooxygenase

Nag, Bishwajit; Dey, Debendranath; Medicherla, Satyanarayana; Neogi, IN Partha

PΑ Theracos, Inc., USA

SO U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U.S. Ser. No. 785,554. CODEN: USXXCO

LΑ	Patent English CNT 12	,				
	PATENT NO.		KIND		APPLICATION NO.	DATE
ΡI	US 20020322 US 7105552			20020314	US 2001-843167	20010427
•	US 6245814		В1	20010612	US 1998-74925	19980508
					US 2001-785554	
	CA 2410171		A1	20011220	CA 2001-2410171	20010605
	WO 20010958	59	A2	20011220	WO 2001-US17950	20010605
	WO 20010958	59	A3	20030828		
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	CO,	CR, C	U, CZ,	DE, DK, DM,	DZ, EC, EE, ES, FI, GB	, GD, GE, GH,
	•	•			JP, KE, KG, KP, KR, KZ	
		-			MK, MN, MW, MX, MZ, NO	
					SL, TJ, TM, TR, TT, TZ	, UA, UG, US,
	•	•	U, ZA,			
					SL, SZ, TZ, UG, ZW, AM	
					CH, CY, DE, DK, ES, FI	
					TR, BF, BJ, CF, CG, CI	, CM, GA, GN,
				SN, TD, TG	NI 2001 66670	20010605
					AU 2001-66670 EP 2001-944241	
					GB, GR, IT, LI, LU, NL	
		FI, C		DR, 65, FR,	GB, GR, 11, 11, 10, NL	, 3B, MC, FI,
	JP 20045274	-		20040909	JP 2002-510041	20010605
				20041013		
				20050527		
	US 20031814	94	A1	20030925	US 2002-265902	_ · · · · · · · · ·

	MX 2002PA12038	Α	20031015	MX 2002-PA12038	20021205
	US 2004186299	A1	20040923	US 2004-808519	20040325
	US 7202366	B2	20070410		
PRAI	US 1998-74925	A2	19980508		
	US 1999-287237	A2	19990406		
	US 2000-591105	A2	20000609		
	US 2001-785554	A2	20010220		
	US 2001-843167	A	20010427		
	WO 2001-US17950	W	20010605		
os	MARPAT 136:247571				
GI					

$$Q = \begin{pmatrix} A_p \\ B_{p1} \\ R \end{pmatrix} \begin{pmatrix} A_q \\ R \end{pmatrix} \begin{pmatrix} A_p \\ Q^1 \\ B_{p1} \end{pmatrix} \begin{pmatrix} R \\ R \end{pmatrix}$$

AB Novel diphenylethylene compds. and derivs. thereof containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes. The above compds. and their derivs. are resented by formula [I; Z = Q, Q1, H, A", B"; wherein n, m, q, q1 = integers from zero to 4 provided that $n+m\le 4$ and $q+q1\le 4$; p, p1 = integers from zero to 5 provided that p+p1≤5; a, b and c are double bonds which may be present or absent; when present; the double bonds may be in the E or Z configuration and, when absent, the resulting stereocenters may have the R- or Sconfiguration; R, R', R" = H, C1-20 linear or branched alkyl, C2-20 linear or branched alkenyl, CO2Z' (wherein Z' = H, Na, K, or other pharmaceutically acceptable counterion such as Ca, Mg, ammonium, tromethamine, and the like), CO2R''', NH2, NHR''', N(R''')2, OH, OR''', halo, substituted C1-20 linear or branched alkyl or substituted C2-20 linear or branched alkenyl (wherein R''' is C1-20 linear or branched alkyl or linear or branched alkenyl); A, A', A'' = H, C1-20 acylamino, C1-20 acyloxy, C1-20 alkanoyl, C1-20 alkoxycarbonyl, C1-20 alkoxy, C1-20 alkylamino, C1-20 alkylcarboxylamino, CO2H, cyano, halo, HO; B, B', B'' = H, C1-20 acylamino, C1-20 acyloxy, C1-20 alkanoyl, C1-20 alkenoyl, C1-20 alkoxycarbonyl, C1-20 alkoxy, C1-20 alkylamino, C1-20 alkylcarboxylamino, aroyl, aralkanoyl, CO2H, cyano, halo, HO; or A and B together, or A' and B' together, or A'' and B'' together, may be joined to form a methylenedioxy or ethylenedioxy group; and X, X' are independently -NH, -NR''', O or S]. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. They inhibit the activity of TNF-alpha, interleukin IL-1 or IL-6 or cyclooxygenase-2 (COX-2). The

compds. are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis. Thus, To a mixture of 3,5-dimethoxybenzaldehyde (500 g) and p-hydroxyphenylacetic acid (457 g) was added acetic anhydride (1 L) and triethylamine (420 mL) and the nonhomogeneous mixture on heating became homogeneous at 70° and stirred at 130-140° for 6 h to give 47% 3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid (II) (428 g). II (427.5 g) was suspended in 3 L methanol, treated with 100 mL concentrated H2SO4, and heated at reflux for 20 h under Ar to give 97% 3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid Me ester (III). III (433 q) was dissolved in 1.6 L DMF, treated with 60.4 q NaH (50% in oil) and the with 185 mL p-fluorobenzaldehyde, and heated at 180° for 18 h to give 77% 3-(3,5-dimethoxyphenyl)-2-[4-(4formylphenoxy)phenyl]acrylic acid Me ester which (352 g), 2,4-thiazolidinedione 98.6, benzoic acid 134, and piperidine 107.4 g were heated in 2.5 L toluene at reflux with continuous removal of H2O through Dean-Stark apparatus to give 86% 3-(3,5-dimethoxyphenyl)-2-[4-[4-(2,4-dimethoxyphenyl)]dioxothiazolidin-5-ylidenemethyl)phenoxy]phenyl]acrylic acid Me ester (IV). IV (30 q) was hydrogenated over 15 q 10% Pd-C in 900 mL dioxane in a Parr apparatus at 60 Psi for 24 h, followed by adding 15 g 10% Pd-C and continuing the hydrogenation for another 24 h to give 86% 3-(3,5-dimethoxyphenyl)-2-[4-[4-(2,4-dioxothiazolidin-5ylmethyl)phenoxy]phenyl]acrylic acid Me ester (V). When V was orally administered to ob/ob mice with a single oral dose (50 mg/kg body weight), there was a 62 % drop in blood glucose level and, similar to db/db mice, there was no significant increase in body weight between the control and the treatment groups. This was in contrast to treatment of diabetic animals by thiazolidinedione type compds. which are known to be associated with increase in body weight

IT 380881-43-6P, 3-(3,5-Dimethoxyphenyl)-2-(4-hydroxyphenyl)propionic acid methyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of novel heterocyclic analogs of phenylethylene compds. as inhibitors of cytokines or cyclooxygenase for therapeutic agents)

RN 380881-43-6 CAPLUS

CN Benzenepropanoic acid, α -(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (CA INDEX NAME)

RE.CNT 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:11108 CAPLUS

DN 136:69654

TI Preparation of diphenylethylene compounds as antidiabetic agents

IN Nag, Bishwagit; Dey, Debendranath; Medicherla, Satyanarayana; Neogi, Partha

PA USA

SO U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 642,618.

CODEN: USXXCO

DT Patent LA English

FAI	N.CNT 12				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PΙ	US 2002002200	A1	20020103	US 2001-777551	20010205
	US 6624197	B1	20030923	US 2000-642618	20000817
	US 2004097593	A1	20040520	US 2003-430677	20030507
	US 2007259961	A9	20071108		
	US 2004259938	A1	20041223	US 2003-690844	20031023
PR	AI US 2000-180340P	P	20000204		
	US 2000-642618	A2	20000817		
	US 1998-74925	A2	19980508		
	US 1999-436047	A3	19991108		
	US 2001-777551	B2	20010205		
	US 2001-334818P	P	20011129		
	US 2002-75442	A2	20020215		
	WO 2002-US38150	A2	20021127		
OS GI	MARPAT 136:69654				

$$R^{2}$$
 R^{3}
 R^{4}
 R^{6}
 R^{5}

AB Title compds. I [wherein A = CO2R, CONR'R", CN, or COR7; X = H, OH, or (un) substituted alkyl or alkenyl; R = H, (ar) alkyl, or aryl; R1, R2, R3, R4, R5, R6, and R7 = independently H, (un) substituted alkyl or alkenyl; CO2R, NR'R", or CONCR'R"; R' and R" = independently H, alkyl, aryl, OH, alkoxy, acylamino, acyloxy, alkanoyl, alkoxylcarbonyl, halo, NO2, SO2R'''; CZ3; Z = independently H, halo, (halo)alkyl, or SR'''; R''' = H or alkyl; or R2 and R3 together or R5 and R6 together may be joined to form (m)ethylenedioxy; with provisos; and E and Z isomers thereof] were prepared and shown to decrease circulating concns. of glucose when administered orally. For instance, 3,5-dimethoxybenzaldehyde was coupled with p-hydroxyphenyl acetic acid using TEA in acetic anhydride to give (E)-3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid (II), which exhibited glucose-lowering effects for more than 15 days at a dose of 20 mg/kg p.o. Examples also include twenty-six bioassays, such as studies on the effects of II on insulin resistant rats, lipid and leptin concns., PPAR binding, overexpression of the human insulin-like growth factor 1 receptor and human insulin receptor, toxicity, and kinetics of drug absorption. I are orally effective antidiabetic agents that normalize glucose and lipid metabolism

IT 353228-00-9P

RN

CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and testing of diphenylethylene antidiabetic agents that normalize glucose and lipid metabolism in relation to insulin resistance) 353228-00-9 CAPLUS

Benzenepropanoic acid, α -(4-hydroxyphenyl)-3,4-dimethoxy- (CA INDEX

NAME)

$$\begin{array}{c|c} \text{OMe} & \text{OMe} \\ \text{CO}_2\text{H} & \text{OMe} \\ \text{CH-CH}_2 & \text{OMe} \end{array}$$

WO 2001-US17950

MARPAT 136:37596

OS

GI

W

20010605

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L7
     ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
     2001:923567 CAPLUS
AN
DN
     136:37596
ΤI
     Preparation and activity of diphenylethylene thiazolidinedione or
     oxazolidinedione compounds as antidiabetics or antiinflammatories
IN
     Neogi, Partha; Nag, Bishwajit; Medicherla, Satyanarayana; Dey,
     Debendranath
PA
     Calyx Therapeutics, Inc., USA
SO
     PCT Int. Appl., 76 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 12
     PATENT NO.
                          KIND
                                             APPLICATION NO.
                                                                     DATE
                                 DATE
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.PI
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     WO 2001095859
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
             RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
             UZ, VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG,
             KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR,
             IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
             GW, ML, MR, NE, SN, TD, TG
     US 2002025975
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                                 20050527
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                                                                     20021204
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     US 2001-843167
                           A2
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     US 1998-74925
                           A2
                                 19980508
     US 1999-287237
                           A2
                                 19990406
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AB Novel diphenylethylene compds. and derivs. thereof containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. Thus, (I) was prepared in five steps by condensation of 3,5-dimethoxybenzaldehyde with 4-hydroxyphenylacetic acid followed by esterification and etherification with 4-fluorobenzaldehyde and condensation with 2,4-thiazolidinedione and hydrogenation of the ylidene double bond. Oral administration of I to obese mice caused a 62% drop in blood glucose level. The compds. are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis.

IT 380881-43-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and activity of diphenylethylene thiazolidinedione or oxazolidinedione compds. as antidiabetics or antiinflammatories)

RN 380881-43-6 CAPLUS

CN Benzenepropanoic acid, α -(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (CA INDEX NAME)

L7 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2001:581654 CAPLUS

DN 135:147444

TI Novel diphenylethylene compounds

IN Nag, Bishwajit; Dey, Debendranath; Medicherla, Satyanarayana

PA Calyx Therapeutics, Inc., USA

SO PCT Int. Appl., 55 pp.

CODEN: PIXXD2

DT Patent

LA English FAN.CNT 12

	PAT	PATENT NO.				KIND DATE			APPLICATION NO.					DATE				
ΡI	WO 2001056382			A1 20010809			WO 2001-US3797						20010205					
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
			CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,
			HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,
									MN,									
									TJ,							-		
				ZA,		•	•		·		•	•	•	•	,	,	•	•
		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,
									GR,									
									GN,								•	•
	US	6624	197			B1		2003	0923		US 2	000-	6426	18	-	2	0000	817
	CA	2397	076			A1												
						20021030		EP 2001-905454						20010205				
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			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR						
	JP 2003521500		Т		20030715 JP 2001-556			5560	90	20010205								
	NZ	5208	29			Α		2004	1224		NZ 2	001-	5208	29		2	0010	205
	ΑU	7849	74			B ₂			0810								0010	205
	MX	2002	PA07	514		A											0020	802
	IN	N 2002CN01321				Α		2007	0309		IN 2	002-	CN13:	21		2	0020	822
PRAI	US	2000	-180	340P		P		2000	0204									
	US	2000	-642	618		A		2000	0817									
	US	1998	-749	25		A2		1998	0508									
		2001						2001	0205									
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OS MARPAT 135:147444

AB Novel diphenylethylene compds. that are administered orally to decrease circulating concns. of glucose are provided. The effect on insulin resistant rats is also shown. The effects on lipid and leptin concns. are also shown. The compds. are orally effective anti-diabetic agents that may normalize glucose and lipid metabolism in subjects with diabetes.

IT 353228-00-9P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(novel diphenylethylene compds. that are anti-diabetic agents that normalize glucose and lipid metabolism in relation to insulin resistance) 353228-00-9 CAPLUS

CN Benzenepropanoic acid, α -(4-hydroxyphenyl)-3,4-dimethoxy- (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} & \text{OMe} \\ \hline \\ \text{CO}_2\text{H} & \text{OMe} \\ \hline \\ \text{CH-CH}_2 & \text{OMe} \\ \end{array}$$

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1999:771171 CAPLUS

DN 132:122418

RN

TI Synthesis and biological evaluation of dihydrobenzofuran lignans and related compounds as potential antitumor agents that inhibit tubulin polymerization

AU Pieters, Luc; Van Dyck, Stefaan; Gao, Mei; Bai, Ruoli; Hamel, Ernest;

Vlietinck, Arnold; Lemiere, Guy

CS Department of Pharmaceutical Sciences, University of Antwerp, Belgium, B-2610, Belg.

Ι

SO Journal of Medicinal Chemistry (1999), 42(26), 5475-5481 CODEN: JMCMAR: ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

GI

AB A series of 19 related dihydrobenzofuran lignans and benzofurans was obtained by a biomimetic reaction sequence involving oxidative dimerization of p-coumaric, caffeic, or ferulic acid Me esters, followed by derivatization reactions. All compds. were evaluated for potential anticancer activity in an in vitro human disease-oriented tumor cell line screening panel that consisted of 60 human tumor cell lines arranged in nine subpanels, representing diverse histologies. Leukemia and breast cancer cell lines were relatively more sensitive to these agents than were the other cell lines. Me (E)-3-[2-(3,4-dihydroxyphenyl)-7-hydroxy-3methoxycarbonyl-2,3-dihydro-1-benzofuran-5-yl]prop-2-enoate (I), the dimerization product of caffeic acid Me ester, containing a 3',4'-dihydroxyphenyl moiety and a hydroxyl group in position 7 of the dihydrobenzofuran ring, showed promising activity. The average GI50 value (the molar drug concentration required for 50% growth inhibition) of I was 0.3 μM . Against three breast cancer cell lines, I had a GI50 value of <10 nM. Methylation, reduction of the double bond of the C3-side chain, reduction

οf

the methoxycarbonyl functionalities to primary alcs., or oxidation of the dihydrobenzofuran ring to a benzofuran system resulted in a decrease or loss of cytotoxic activity. Compound I inhibited mitosis at micromolar concns. in cell culture through a relatively weak interaction at the colchicine binding site of tubulin. In vitro it inhibited tubulin polymerization

by 50% at a concentration of 13 \pm 1 $\mu M.$ The 2R,3R-enantiomer of I was twice as active as the racemic mixture, while the 2S,3S-enantiomer had minimal activity as an inhibitor of tubulin polymerization. These dihydrobenzofuran lignans (2-phenyl-dihydrobenzofuran derivs.) constitute a new group of antimitotic and potential antitumor agents that inhibit tubulin polymerization

IT 256330-13-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and biol. evaluation of dihydrobenzofuran lignans and related compds. as potential antitumor agents that inhibit tubulin polymerization)

RN 256330-13-9 CAPLUS

CN Benzenepropanoic acid, α -[2-hydroxy-3-methoxy-5-(3-methoxy-3-oxopropyl)phenyl]-3,4-dimethoxy-, methyl ester (CA INDEX NAME)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1966:429366 CAPLUS

DN 65:29366

OREF 65:5434e-f

TI Flavanoids. II. Stereochemistry of isoaurones

AU Marathe, K. G.; Byrne, M. J.; Vidwans, R. N.

CS Univ. Poona, India

SO Tetrahedron (1966), 22(6), 1789-95

CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

AB cf. CA 54, 3402a. Isoaurones (anhydrolactones of 2-hydroxy- α -benzylmandelic acids), trimethylanhydrohazeyl lactone and its 5-methyl-4'-methoxy analog are shown to be trans-stilbene derivs. and are isomerized to the cis compds. by pyridine. The stereochemistry has been established by a stereoselective synthesis of the derived cis-stilbene- α -carboxylic acid and confirmed by uv and N.M.R. studies. A mechanism for isomerization has been suggested.

IT 6600-62-0P, Lactic acid, 3-(3,4-dimethoxyphenyl)-2-(2-hydroxy-4-methoxyphenyl)-

RL: PREP (Preparation)

(preparation of)

RN 6600-62-0 CAPLUS

CN Lactic acid, 3-(3,4-dimethoxyphenyl)-2-(2-hydroxy-4-methoxyphenyl)- (7CI, 8CI) (CA INDEX NAME)

L7 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1966:93097 CAPLUS

DN 64:93097

OREF 64:17468f-h,17469a-b

TI Reaction of 2,6-and 2,4-xylenols with oxo acids

```
AU
    Merchant, J. R.; Mehta, J. B.
CS
     Inst. Sci., Bombay
SO
     Indian Journal of Chemistry (1966), 4(2), 76-8
     CODEN: IJOCAP; ISSN: 0019-5103
DT
     Journal
     English
LΑ
GI
     For diagram(s), see printed CA Issue.
AB
     cf. Parris, et al., CA 57, 723i; Smith and Bealor, CA 57, 12377q. Concentrated
    H2SO4 (5 ml.) was added dropwise with stirring to a mixture of 4.8 q.
     2,6-xylenol (I) and 1.76 g. pyruvic acid kept at 0-5°. After 30
     min., the mixture was poured into ice-cold H2O to yield 3 q.
     2,2-bis(3,5-dimethyl-4-hydroxyphenyl)propionic acid (II), m.
     201-2°. II was also obtained when dry HCl was passed through a
     mixture of the same amounts of the reactants in 10 ml. HOAc at 0-5°
     for 4 hrs. Similarly, condensation of 2.4 g. I with 1.64 g. phenylpyruvic
     add, 2.2 g. 3,4-dimethoxyphenylpyruvic acid, 1 g. dimethylpyruvic acid, 1
     g. \alpha-oxo-n-valeric acid, and 1.5 g. \alpha-oxoglutaric acid, resp.,
     in HOAc at 0-5^{\circ} in the presence of HCl yielded 2 g.
     2,2-bis(3,5-dimethyl-4-hydroxyphenyl)phenylpropionic acid, m.
     239-40° (C6H6); 1 g. 2,2-bis(3,5-dimethyl-4-hydroxyphenyl)-
     3,4-dimethoxyphenylpropionic acid, m. 190-1° (dilute EtOH); 450 mg.
     2,2-bis(3,5-dimethyl-4-hydroxyphenyl)dimethylpropionic acid, m.
     250-1° (C6H66); 2,2-bis(3,5-dimethyl-4-hydroxy-
    phenyl)propylpropionic acid, m. 235-6° (C6H6); and 1 g. 2,2-
    bis(3,5-dimethyl-4-hydroxyphenyl)glutaric acid (III), m. 208-9°
     (EtOAc-petr. ether). Esterification of III by refluxing 12 hrs. with EtOH
     saturated with HCl yielded the ester, m. 158-9° (EtOAc). On refluxing
     2 hrs. with Ac20, III yielded the corresponding anhydride, m.
     230-1° (C6H6-petr. ether). Dry HCl was passed 6 hrs. at
     0-5° through a mixture of 2.4 g. I, 1.2 ml. MeCOCH2CO2Et, and 10 ml.
    HOAc and the mixture kept overnight to yield 1.7 g. Et 3,3-bis(3,5-dimethyl-
     4-hydroxyphenyl)butanoate, m. 147-8° (C6H6-petr. ether). Attempted
    condensation of 2.4 g. I with 1.3 g. Et 2-methylacetoacetate in 10 ml.
    HOAc in the presence of HCl yielded a product, m. 192-3° (EtOAc),
    which could not be characterized. Similar condensation of 2.4 g. I and 2
    ml. ethyl acetonedicarboxylate yielded 400 mg. 2,2-bis(4-hydroxy-3,5-
     dimethylphenyl)propane, m. 161-2°. The reaction of 2,4-xylenol
     (IV) with diethyl oxalacetate Na salt in the presence of concentrated H2SO4 at
     0° yielded a crystalline neutral solid (V), which was identical with
     that obtained by Smith and Bealor (loc. cit.). Concentrated H2SO4 (10 ml.) was
    added dropwise with stirring to a previously cooled (0-5°) mixture of
     2.4 g. IV and 2 ml. ethyl acetonedicarboxylate and the mixture kept
    overnight to yield 1 g. 4-carboxymethyl-6,8-dimethylcoumarin (VI), m.
     206-7°, and 1 g. 4-carbethoxymethyl-6,8-dimethylcoumarin (VII), m.
     100° (EtOAc-petr. ether).
ΙT
    5613-39-8
        (Derived from data in the 7th Collective Formula Index (1962-1966))
RN
    5613-39-8 CAPLUS
CN
    Propionic acid, 3-(3,4-dimethoxyphenyl)-2,2-bis(4-hydroxy-3,5-xylyl)-
     (7CI, 8CI) (CA INDEX NAME)
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L7 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN AN 1966:93096 CAPLUS DN 64:93096 OREF 64:17468d-f
TI Highly pure hippuran-1311

AU Charamza, Otakar; Opavsky, Jiri

CS Fakultni Nemocnice, Olomouc, Czech.

SO Vnitrni Lekarstvi (1965), 11(12), 1211-15

CODEN: VNLEAH; ISSN: 0042-773X

DT Journal LA Czech

AB o-Iodohippuric acid (I) is obtained from o-H2NC6H4CO2H
(II) via o-IC6H4CO2H (III) and yields 90% labeled I by ion
exchange with Na13II and isolation on a column containing AgCl-sea sand.
Thus, a mixture of 30.3 ml. 96% H2SO4, 100 ml. H2O, and 25 g. II is treated
at 0° dropwise in 1 hr. with a solution of 12.6 g. NaNO2 in 50 ml.
H2O, the brownish solution stirred 30 min. at 0° and 30 g. KI in 50
ml. H2O added with cooling discontinued. The mixture is kept 16 hrs.,
heated at 60° 30 min. with stirring, shaken with Et2O, the product
taken up with dilute NaOH, precipitated with HCl, and recrystd. from H2O to
give 20

g. III, m. 160-1°. III (10 g.) is refluxed at 80° with fresh SOC12 until evolution of SO2 has ceased (45 min.), the SOC12 distilled in vacuo and with excess C6H6, the residue in C6H6 added dropwise to a mixture of 3 g. H2NCH2CO2H, 2 g. NaOH, and 15 ml. H2O, the mixture stirred 20 min. at <30° with addition of NaOH solution to keep neutral, cooled, and made acid to yield 8.6 g. I, m. 171-4° (H2O). I (0.01-0.1 g.) and 0.1 ml. 0.2% KI is treated in a rubber-stoppered vial with the corresponding amount of Na131I added from a syringe, the mixture kept 2 hrs. in a boiling H2O bath and neutralized at 30-40° with 0.5N NaHCO3. The solution is transferred by means of the syringe onto a column of AgCl-sea sand (1 g.:2 g.) which is then rinsed with 3 ml. physiol. saline. The preparation contains 0.2-0.3 mc./ml. (50 μ c./mg.) and is ready for use in reno-, splenoporto-, and cerebral circulography after sterilization.

IT 5613-39-8

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 5613-39-8 CAPLUS

CN Propionic acid, 3-(3,4-dimethoxyphenyl)-2,2-bis(4-hydroxy-3,5-xylyl)-(7CI, 8CI) (CA INDEX NAME)

L7 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1966:91549 CAPLUS

DN 64:91549

OREF 64:17168e-h

TI Properties and structure of titanium bronzes containing from 0.17 to 5.26 weight % Ti, melted in an induction furnace without the application of an inert atmosphere

AU Gebalski, Stanislaw; Przygodzki, Wieslaw

SO Prace Inst. Mech. Precyzyjnej (1962), 10(4), 23-42

DT Journal

LA Polish

AΒ Five alloys (Cu-Ti) containing 0.17, 1.72, 2.45, 4.25, and 5.26 weight % Ti and impurities 0.5%, rest Cu were melted in an induction furnace in silica-graphite crucibles of capacity 20 kg. with 225,000 frequency and 30 w. power. Copper (Cu 99.9%) was preheated to 500-600° and the flux was introduced whereupon the Cu was melted and heated to 1200°. Afterwards the alloy Cu-Ti with 16.21 weight % Ti was introduced and the temperature was raised to 1250-1300°. The slag was then thickened by the addition of fluorite. The slag was poured off and the alloy was cast at 1260 ± 20° into preheated (to 200°) molds. The ingots were cooled in air, and then placed in stainless steel boxes and packed with charcoal. The protected ingots were then placed into a preheated furnace where they were heated for 6 h. at 900°. The ingots were then cooled in water at 15° then aged for 25 h. at 450°, and cooled in air. Thereafter the tensile strength, elongation, contraction, hardness and microhardness, modulus of elasticity, and coefficient of linear expansion were determined Optimum properties were exhibited by the Cu-Ti alloy containing 2.25-4.25 weight % Ti. A higher content of Ti leads to brittleness without much increase in tensile strength and hardness. The alloys containing 2.45 and 4.25% Ti had after aging the following properties: tensile strength in kg./mm.2, 66 and 75; hardness in kg./mm.2 240 and 200; elongation in 16% and 5, Young's modulus in kg./mm.2, 11,800 and 12,000. The melting of Cu-Ti alloys in air in an induction furnace should be done under a flux which should be thickened; otherwise the metal will contain too high a content of oxide inclusions, and the burn off of Ti will be excessive. The optimum aging conditions were 2 h. at 450° or 8 h. at 430°. 18 refs.

IT 5613-39-8P, Propionic acid, 3-(3,4-dimethoxyphenyl)-2,2-bis(4hydroxy-3,5-xylyl)-

RL: PREP (Preparation)

(preparation of)

RN 5613-39-8 CAPLUS

CN Propionic acid, 3-(3,4-dimethoxyphenyl)-2,2-bis(4-hydroxy-3,5-xylyl)-(7CI, 8CI) (CA INDEX NAME)

8CI) (CA INDEX NAME)

L7ANSWER 12 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN AN 1935:6099 CAPLUS DN 29:6099 OREF 29:762a-g TI Constitution of fustin. II and III. The constitution of hazeic acid (1 and ΑU Oyamada, Taichiro SO Nippon Kagaku Kaishi (1921-47) (1934), 55, 763-74,775-85 CODEN: NIKWAB; ISSN: 0369-4208 DT LΑ Unavailable GI For diagram(s), see printed CA Issue. AB No crystalline product is obtainable from fustin (I) by treating it with dilute acid or alkali, but when methylfustin (II), m. 142-3°, obtained by methylation of I with CH2N2, is treated with dilute alkali, it gives trimethylhazeic acid (III). II with alkali gives 10-20% of 7,3',4'-trimethoxy-3-hydroxyflavone (IV), m. 184-5°, and 40% III, colorless column, m. 138°. III with CH2N2 gives Me tetramethylhazeinate (V), m. 171-2°. V gives tetramethylhazeic acid (VI), m. 188-90°, with dilute alkali, and VI gives V with CH2N2. V and VI are also obtainable by methylation of I with Me2SO4 and alkali (yield 10-40%). III with acid gives anhydrotrimethylhazeyl lactone (VII), C18H16O5, yellow crystals, m. 185°. VII gives anhydrotrimethylhazeic acid (VIII), C18H18O6, on heating several hrs. with alkali. VIII gives Me anhydrotetramethylhazeinate, m. 116°, by diazotation with CH2N2. VI gives a ketone (IX), m. 98.5-9.5°, by the oxidation with KMO4 and the fusion of VI gives anhydrotetramethylhazeic acid, m. 166-8°. The above facts indicate that VI is an αHO acid having 2 C6H6 nuclei and at least one of the C next to C holding the OH group is not tertiary. The phenolic OH group is in such a position as to form a stable lactone with CO2H; 4 of the O atoms must be in phenolic OH groups since they can easily be methylated by CH2N2 or Me2SO4 and demethylated by HI. The constitution of VI is expressed by 1 of the following formulas: Accordingly III must be VI in which 1 of the 4 OMe groups is replaced by OH. IX gives an oxime (X), C18H21O5N, m. 134-6°, with NH2OH-HCl and alc. KOH. X can be transformed into an amide (XI), m. 120-2°, by PCl5. Saponification of XI gives a homoveratric acid, m. 96-8°, and a dimethoxyaniline, m. 36-8°, which is closest to 2,4-(MeO)2C6H3NH2. The constitution of hazeic acid, therefore, is [2,4-(HO)2C6H3][3,4-(HO)2C6H8CH2] C(OH)CO2H. IT 6600-62-0P, Hazeic acid, trimethyl-RL: PREP (Preparation) (preparation of) RN 6600-62-0 CAPLUS CN Lactic acid, 3-(3,4-dimethoxyphenyl)-2-(2-hydroxy-4-methoxyphenyl)- (7CI,

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AN 1979:203702 CAPLUS

DN 90:203702

OREF 90:32393a,32396a

TI 5-Oxopentanoic acid derivatives

IN Fisnerova, Ludmila; Nemecek, Oldrich; Grimova, Jaroslava

PA Czech.

SO Czech., 6 pp.

CODEN: CZXXA9

DT Patent

LA Czech

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI CS 176744	B1	19770630	CS 1975-2824	19750423	
PRAT CS 1975-2824	Δ	19750423	•		

GI

The title compds. I (R1 = H, C3-4 alkyl, C1, NO2, OMe; R2 = H, CHMe2, NMe2, C1, NO2; R3 = Ph, 2-furyl, CMe3, 3-indanyl, C6H3C12-2,4) were prepared by addition of 4-R1C6H4CH2CO2Et to 4-R2C6H4CH:CHCOR3 and saponification of the product. Thus, a solution of 2.46 g PhCH2CO2Et and 3.7 g 4-Me2CHC6H4CH:CHCOPh in Et2O containing EtONa was kept 5 days to give 4.4 g PhCOCH2CH(C6H4CHMe2-4)CHPhCO2Et which was refluxed with AcOH-HBr to yield 3.5 g I (R1 = H, R2 = CHMe2, R3 = Ph). Similarly prepared were PhCOCH2CHR4CHR5CO2H (R4 = 2-pyrrolyl, 3-pyridyl; R5 = Ph, C6H4NO2-4, C6H4CH2CHMe2-4).

IT 59771-47-0P 59771-91-4P 70334-43-9P 70334-44-0P 70334-45-1P 70334-46-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 59771-47-0 CAPLUS

CN Benzenepentanoic acid, β -[4-(1-methylethyl)phenyl]- α -[4-(1-methylpropyl)phenyl]- δ -oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 59771-91-4 CAPLUS

CN Benzenepentanoic acid, β -[4-(1-methylethyl)phenyl]- α -[4-(1-methylpropyl)phenyl]- δ -oxo-(9CI) (CA INDEX NAME)

$$CH_2-C-Ph$$
 CO_2H
 $CH-CH-CH$
 $CH-Et$
 Me

RN 70334-43-9 CAPLUS

CN Benzenepropanoic acid, β -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- α -[4-(2-methylpropyl)phenyl]-, ethyl ester (CA INDEX NAME)

RN 70334-44-0 CAPLUS

CN Benzenepropanoic acid, β -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- α -[4-(2-methylpropyl)phenyl]- (CA INDEX NAME)

RN 70334-45-1 CAPLUS

CN Benzenepropanoic acid, β -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- α -[4-(1-methylethyl)phenyl]-, ethyl ester (CA INDEX NAME)

RN 70334-46-2 CAPLUS

CN Benzenepropanoic acid, β -(3,3-dimethyl-2-oxobutyl)-4-(1-methylethyl)- α -[4-(1-methylethyl)phenyl]- (CA INDEX NAME)

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ANSWER 128 OF 267 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1985:45575 CAPLUS

DN 102:45575

OREF 102:7157a,7160a

TI Synthetic studies in polycyclic systems: part IX - synthesis of methoxy derivatives of 11H-benzo[a]fluorenes and 11H-naphtho[2,1-a]fluorenes

AU Rao, Alaka; Lala, Sunandan; Rao, R. R.

CS Dep. Chem., Visva-Bharati Univ., Santiniketan, 731 235, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(7), 603-10

CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

OS CASREACT 102:45575

GΙ

$$R^{2}$$
 R^{3}
 R^{2}
 R^{2}
 R^{3}
 R^{2}
 R^{3}
 R^{2}
 R^{3}
 R^{4}
 R^{5}
 R^{6}
 R^{1}

Michael reaction of RCH:CHCO2Et [R = C6H4OMe-2, -3, -3, C6H3COMe)2-3,4] with R1CH2CO2Et (R1 = Ph, 2-naphthyl) gave 75-86% EtO2CCHR1CHRCH2CO2Et, which was hydrolyzed to give HO2CCHR1CNRCH2CO2H. The diacids were cyclized with SnCl4 to give 54-64% tetralone derivs. I (R2 = R3 = H, CH:CHCH:CH; X = O) which were reduced with Zn or H2NNH2 to give 58-67, 59-66% I (X = H2) resp. The last were methylated, dehydrogenated, and saponified to give naphthalene- and phenanthrenecarboxylic acids II (same R's), which were cyclized using H2SO4, AlCl3, or SnCl4 to give 18-38, 29-42, 52-74% fluorenone derivs. III (R4 = R6 = OMe, R3 = H; R4 = OMe, R5 = R6 = H; R4 = R6 = H, R5 = OMe; R4 = R5 = H, R6 = OMe, X6 = O), resp. The ketones were reduced with H2NNH2 to give 54-67% title compds. III (same R's, X1 = H2).

IT 94146-62-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and saponification of)

RN 94146-62-0 CAPLUS

IT 94146-18-6P 94146-19-7P 94146-20-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 94146-18-6 CAPLUS

CN Pentanedioic acid, 2-(2-carboxyphenyl)-3-(3-methoxyphenyl)- (CA INDEX NAME)

RN 94146-19-7 CAPLUS

CN Pentanedioic acid, 2-(2-carboxyphenyl)-3-(4-methoxyphenyl)- (CA INDEX NAME)

RN 94146-20-0 CAPLUS

CN Pentanedioic acid, 2-(2-carboxyphenyl)-3-(3,4-dimethoxyphenyl)- (CA INDEX NAME)

IT 94146-63-1P 94146-64-2P 94146-65-3P

94146-66-4F

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, hydrolysis, and Dieckmann cyclization of)

RN 94146-63-1 CAPLUS

CN Pentanedioic acid, 2-[2-(ethoxycarbonyl)phenyl]-3-(3-methoxyphenyl)-, diethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

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(FILE 'HOME' ENTERED AT 08:08:15 ON 27 DEC 2007)

FILE 'REGISTRY' ENTERED AT 08:08:27 ON 27 DEC 2007

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 1 S L1 CSS

L4 1 S L1 CSS FUL

=> d ide bib 14

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 353228-00-9 REGISTRY

ED Entered STN: 28 Aug 2001

CN Benzenepropanoic acid, α -(4-hydroxyphenyl)-3,4-dimethoxy- (CA INDEX NAME)

MF C17 H18 O5

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c|c} \text{OMe} & \text{OMe} \\ \hline \text{CO}_2\text{H} & \text{OMe} \\ \hline \text{CH-CH}_2 & \text{OMe} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 136:69654 CA

TI Preparation of diphenylethylene compounds as antidiabetic agents

IN Nag, Bishwagit; Dey, Debendranath; Medicherla, Satyanarayana; Neogi, Partha

PA USA

SO U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 642,618. CODEN: USXXCO

DT Patent

LA English

FAN CNT 12

FAN.CNT 12									
	PATENT NO.	KIND	DATE	API	PLICATION NO.	DATE			
PΙ	US 2002002200	A1	20020103	US	2001-777551	20010205			
	US 6624197	B1	20030923	US	2000-642618	20000817			
	US 2004097593	A1	20040520	US	2003-430677	20030507			
	US 2007259961	A9	20071108						
	US 2004259938	A1	20041223	US	2003-690844	20031023			
PRAI	US 2000-180340P	20000204							
	US 2000-642618	20000	817						
	US 1998-74925	19980	508						
	US 1999-436047	19991							
	US 2001-777551	20010205							
	US 2001-334818P	20011	129						
	US 2002-75442	20020	215						

WO 2002-US38150 20021127

REFERENCE 2

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135:147444
AN
ΤI
    Novel diphenylethylene compounds
    Nag, Bishwajit; Dey, Debendranath; Medicherla, Satyanarayana
IN
     Calyx Therapeutics, Inc., USA
PA
     PCT Int. Appl., 55 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 12
                                         APPLICATION NO. DATE
     PATENT NO.
                     KIND DATE
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                     A1
                           20010809
PΙ
    WO 2001056382
                                         WO 2001-US3797 20010205
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            HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
            LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
            SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
            YU, ZA, ZW
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            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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     CA 2397076
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                                                            20010205
     EP 1251738
                            20021030
                                          EP 2001-905454
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                                                            20010205
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
    JP 2003521500
                            20030715
                                                            20010205
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                                          JP 2001-556090
    NZ 520829
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    AU 784974
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                            20060810
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                                                            20010205
    MX 2002PA07514
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                            20040226
                                          MX 2002-PA7514
                                                            20020802
     IN 2002CN01321
                      Α
                            20070309
                                          IN 2002-CN1321
                                                            20020822
PRAI US 2000-180340P
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     US 2000-642618
                      20000817
    US 1998-74925
                      19980508
    WO 2001-US3797
                      20010205
RE.CNT 7
             THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
             ALL CITATIONS AVAILABLE IN THE RE FORMAT
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